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Simultaneous probe of the charm and bottom quark Yukawa couplings using $t\bar{t}H$ events

The CMS Collaboration*

Abstract

A search for the standard model Higgs boson decaying to a charm quark-antiquark pair, $H \rightarrow c\bar{c}$, produced in association with a top quark-antiquark pair ($t\bar{t}H$) is presented. The search is performed with data from proton-proton collisions at $\sqrt{s} = 13$ TeV, corresponding to an integrated luminosity of 138 fb^{-1} . Advanced machine learning techniques are employed for jet flavor identification and event classification. The Higgs boson decay to a bottom quark-antiquark pair is measured simultaneously and the observed $t\bar{t}H(H \rightarrow b\bar{b})$ event rate relative to the standard model expectation is $0.91^{+0.26}_{-0.22}$. The observed (expected) upper limit on the product of production cross section and branching fraction $\sigma(t\bar{t}H)\mathcal{B}(H \rightarrow c\bar{c})$ is 0.11 ($0.13^{+0.06}_{-0.04}$) pb at 95% confidence level, corresponding to 7.8 ($8.7^{+4.0}_{-2.6}$) times the standard model prediction. When combined with the previous search for $H \rightarrow c\bar{c}$ via associated production with a W or Z boson, the observed (expected) 95% confidence interval on the Higgs-charm Yukawa coupling modifier, κ_c , is $|\kappa_c| < 3.5$ (2.7), the most stringent constraint to date.

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The discovery of a Higgs boson (H) by the ATLAS [1] and CMS [2, 3] experiments was a landmark achievement in understanding electroweak (EW) symmetry breaking. With a measured mass of 125.38 ± 0.14 GeV [4], the Higgs boson's observed interactions with gauge bosons and third-generation fermions [5–15], as well as all its measured properties [16–24], align with the standard model (SM) predictions. Following the first evidence of Higgs boson decays to muons, i.e., second-generation leptons [25], another important milestone is to observe its couplings to second-generation quarks.

Searches for Higgs boson decays to a charm quark-antiquark pair, $c\bar{c}$, provide direct access to the charm quark Yukawa coupling, y_c . To date, the most sensitive approach at the LHC exploits associated production of a Higgs boson with a V (W or Z) boson. Using proton-proton (pp) collision data at 13 TeV, corresponding to an integrated luminosity of about 140 fb^{-1} , the ATLAS [26] and CMS [27] Collaborations reported observed (expected) 95% confidence level (CL) intervals on $\kappa_c = y_c/y_c^{\text{SM}}$ of $|\kappa_c| < 4.2$ (4.1) and $1.1 < |\kappa_c| < 5.5$ ($|\kappa_c| < 3.4$), respectively. The search in the dominant gluon fusion production mode yields lower sensitivity because of the overwhelming $c\bar{c}$ background from quantum chromodynamics (QCD) multijet production [28]. Despite these advancements, projections for the High-Luminosity LHC [29] indicate that current approaches may prove insufficient to achieve evidence of $H \rightarrow c\bar{c}$ decay within the experiment's lifetime.

In this Letter, we present a new approach: to search for $H \rightarrow c\bar{c}$ via associated production of a Higgs boson with a top quark-antiquark pair ($t\bar{t}H$) and to measure simultaneously the $H \rightarrow b\bar{b}$ decay. We use pp collision data at $\sqrt{s} = 13$ TeV, collected with the CMS detector in 2016–2018, and corresponding to an integrated luminosity of 138 fb^{-1} [30–32]. The analogous processes $t\bar{t}Z(Z \rightarrow c\bar{c})$ and $t\bar{t}Z(Z \rightarrow b\bar{b})$ are measured to validate the analysis strategy. For $t\bar{t}H(H \rightarrow c\bar{c})$ and $t\bar{t}H(H \rightarrow b\bar{b})$, the presence of multiple jets, including several b and c jets, poses significant challenges in identifying the jet origins and in reconstructing the top quark and Higgs boson decays. To address this, we employ advanced machine learning algorithms, PARTICLENET [33] for jet flavor identification and PARTICLE TRANSFORMER (PART) [34] for event classification. The resulting sensitivity is comparable to the best achieved in the VH channel [27].

The CMS apparatus [35, 36] is a multipurpose, nearly hermetic detector, designed to trigger on [37–39] and identify electrons, muons, photons, and hadrons [40–42]. A global “particle-flow” algorithm [43] aims to reconstruct all individual particles in an event, combining information provided by the all-silicon inner tracker and by the crystal electromagnetic and brass-scintillator hadron calorimeters, operating inside a 3.8 T superconducting solenoid, with data from the gas-ionization muon detectors embedded in the flux-return yoke outside the solenoid. The reconstructed particles are used to build jets, employing the anti- k_T algorithm [44, 45] with a distance parameter $R = 0.4$, and to compute missing transverse momentum [46, 47].

Signal and background processes are simulated using various Monte Carlo event generators. The $t\bar{t}H$ signal process is generated at next-to-leading order (NLO) accuracy in QCD using POWHEG v2 [48–50], with the Higgs boson and top quark masses set to 125 and 172.5 GeV, respectively. The main background is $t\bar{t}$ production with additional jets ($t\bar{t} + \text{jets}$), particularly when these additional jets originate from the hadronization of b or c quarks, as such events closely resemble the signal topology. This background is categorized based on the flavor of the additional jets, i.e., those that do not originate from top quark decays. Jets containing at least one b hadron (at least one c hadron and no b hadron) are defined as b (c) jets, following the ghost association procedure [51]. The remaining jets are labeled as light jets. Events containing one extra b jet are labeled as $t\bar{t} + b$, while those with two or more are labeled as $t\bar{t} + \geq 2b$. Similarly, events with no b jets but one (two or more) extra c jet are labeled as $t\bar{t} + c$ ($t\bar{t} + \geq 2c$).

The remaining $t\bar{t}$ +jets events, containing no b or c jets other than those from top quark decays, are labeled $t\bar{t}$ +light. To achieve the highest available accuracy in modeling the $t\bar{t}$ +jets components, a dedicated $t\bar{t}b\bar{b}$ sample is used to predict the $t\bar{t}+b$ and $t\bar{t}+\geq 2b$ backgrounds. This sample is generated at NLO in QCD in the four-flavor scheme using POWHEG-BOX-RES [52, 53] and OPENLOOPS [54], explicitly including additional b quarks in the matrix element calculation. Contributions to $t\bar{t}+b$ and $t\bar{t}+\geq 2b$ from double parton scattering—amounting to $\approx 15\%$ of the $t\bar{t}b\bar{b}$ production cross section—are not included in the $t\bar{t}b\bar{b}$ sample and are modeled separately. The remaining components, $t\bar{t}+c$, $t\bar{t}+\geq 2c$, and $t\bar{t}$ +light, are modeled using an inclusive $t\bar{t}$ sample simulated with POWHEG v2 at NLO in QCD in the five-flavor scheme [55]. Measurements of $t\bar{t}+\geq 1b$ and $t\bar{t}+\geq 1c$ production [56–59] indicate moderate mismodeling in simulation, necessitating corrections of the background estimates based on control samples in data.

Single top quark production in the t channel (s channel) and in association with a W boson is simulated at NLO accuracy with POWHEG v2 [60–62] (MADGRAPH5_AMC@NLO v2.6.5 [63]). The production cross sections for the $t\bar{t}$ and single top quark samples are computed at next-to-NLO (NNLO) [64, 65]. For $t\bar{t}$, the differential cross section as a function of top quark p_T is corrected to the NNLO QCD + NLO EW prediction [66]. The $t\bar{t}W$ and $t\bar{t}Z$ (tWZ) processes are simulated at NLO (leading order, LO) accuracy in QCD using MADGRAPH5_AMC@NLO. The matching of jets from matrix element calculations and those from parton showers is done with the FxFx [67] (MLM [68]) prescription for NLO (LO) samples. For all samples, the proton structure is described by the NNLO NNPDF3.1 parton distribution function (PDF) set [69]. Parton showering and hadronization are handled by PYTHIA v8.240 [70] with the CP5 underlying event tune [71]. Additional pp interactions within the same or nearby bunch crossings (pileup) are simulated with PYTHIA and added to the hard-scattering process, with events reweighted to match the pileup profile observed in data. The detector response is modeled with GEANT4 [72].

The analysis is carried out in three mutually exclusive channels targeting the fully hadronic (0L), single-lepton (1L), and dilepton (2L) decays of the top quark-antiquark pair. Events are collected using triggers based on high jet and b jet multiplicities, or on the presence of one or two well-identified and isolated leptons (electrons or muons). In the offline selection, only jets with transverse momentum $p_T > 25$ GeV and pseudorapidity $|\eta| < 2.4$ are considered. In the 0L channel, events must contain at least seven jets, of which at least six have $p_T > 40$ GeV, and have a jet p_T scalar sum exceeding 500 GeV to satisfy trigger requirements. The 1L channel selects events with one isolated electron or muon with a minimum p_T of 26 to 30 GeV, depending on the lepton flavor and data-taking year, along with at least five jets. The 2L channel selects events with two oppositely charged leptons, at least one with $p_T > 25$ GeV, and at least four jets. To suppress the Drell–Yan background, events with a dielectron or dimuon invariant mass below 20 GeV or within the Z boson mass window (76–106 GeV) are excluded. Across all channels, events must contain at least three jets tagged as either b or c jets, with at least one tagged as a b jet, using criteria corresponding to tagging efficiencies of approximately 70% (50%) for b (c) jets. Additional details of the event selection criteria are provided in Supplemental Material (Section B.3).

A key challenge in this analysis is accurately identifying jet flavor—not only efficiently tagging heavy-flavor jets initiated by b or c quarks but also distinguishing between them. To address this, PARTICLENET [33], a dynamic graph convolutional neural network [74], is employed to classify jet flavors by leveraging spatial and kinematic correlations of individual particles and secondary vertices associated with the jets. Two discriminants are constructed from the PARTICLENET outputs: p_{B+C} , which differentiates heavy-flavor from light jets, and p_{BvsC} , which distinguishes b from c jets. Based on these, 11 mutually exclusive tagging categories are de-

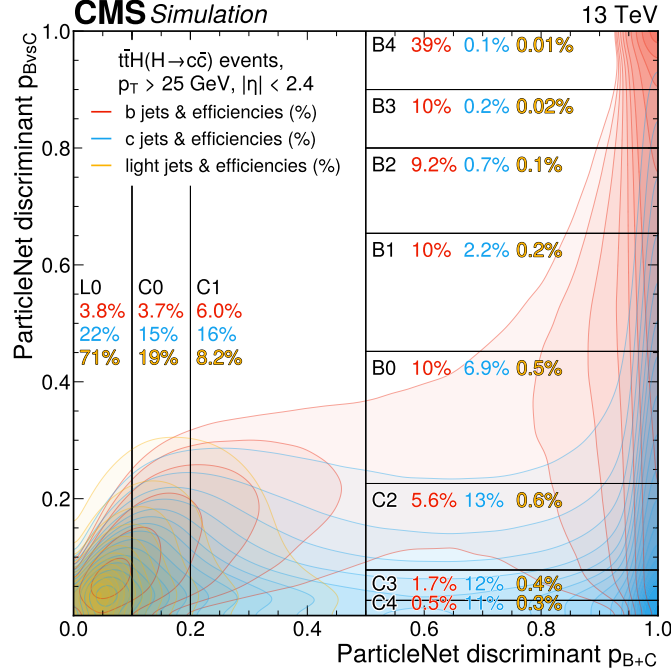


Figure 1: Distribution of b, c, and light jets in the two-dimensional PARTICLENET discriminant plane. The vertical and horizontal lines correspond to the edges of the tagging categories. The numbers in each bin correspond to the tagging efficiencies for b (red), c (blue), and light (yellow) jets, evaluated on a sample of simulated $t\bar{t}H(H \rightarrow c\bar{c})$ events. The contour lines represent constant density values for each jet type in steps of 5%.

defined as shown in Fig. 1: five b-tagging categories (B0–B4), five c-tagging categories (C0–C4), and one untagged category (L0) enriched in light jets. Compared to the previously used DEEPJET algorithm [75], PARTICLENET improves background jet rejection by up to a factor of two at the same signal jet efficiency, demonstrating superior performance in distinguishing jet flavors.

To correct for potential mismodeling of tagging efficiencies in simulation, flavor-dependent scale factors are derived using data samples targeting the production of W +jets, dileptonic $t\bar{t}$, and Z +jets, which are enriched in c, b, and light jets, respectively. These scale factors, defined as data-to-simulation efficiency ratios for each jet type in the 11 tagging categories as functions of jet p_T , are extracted via a simultaneous profile likelihood fit to all three data samples. Further details about the tagger performance and calibration are provided in Supplemental Material (Section B.2). The scale factors typically range from 0.75 to 1.5, with uncertainties of up to $\approx 15\%$ for b jets and up to $\approx 50\%$ for c and light jets.

A further challenge involves distinguishing the $t\bar{t}H$ signal from the $t\bar{t}+$ jets background. Both processes produce numerous jets, including multiple b and c jets, which may originate from top quark or Higgs boson decays, or from additional quark or gluon radiation. This complexity hinders precise jet origin identification and full decay chain reconstruction. To overcome this, a multiclass event classifier based on PART [34] is developed to classify events directly from final-state objects—jets, leptons, and missing transverse momentum—without requiring explicit reconstruction of the top quarks or the Higgs boson. For every object, the classifier receives kinematic inputs in terms of $\ln(p_T/\text{GeV})$, $\ln(E/\text{GeV})$, and η . Jet flavor is encoded via 10 boolean values corresponding to the tagging categories B0–B4 and C0–C4. For each lepton, a flag is included to distinguish between electrons and muons. To better capture event kinematic

values and object correlations, PART constructs pairwise features (e.g., angular separation and invariant mass) for all object pairs using their four-momenta. The classifier is trained to assign likelihood scores across 10 (9) classes in the 0L (1L, 2L) channel:

- Two $t\bar{t}H$ classes: $t\bar{t}H(H \rightarrow c\bar{c})$, $t\bar{t}H(H \rightarrow b\bar{b})$.
- Two $t\bar{t}Z$ classes: $t\bar{t}Z(Z \rightarrow c\bar{c})$, $t\bar{t}Z(Z \rightarrow b\bar{b})$.
- Five $t\bar{t}$ +jets classes: $t\bar{t}+b$, $t\bar{t}+\geq 2b$, $t\bar{t}+c$, $t\bar{t}+\geq 2c$, $t\bar{t}+\text{light}$.
- (Only in the 0L channel) one class for QCD multijet.

The PART classifier is used to refine event selection and categorization. In the 0L channel, a stringent requirement on the QCD multijet discriminant suppresses this background by nearly four orders of magnitude, allowing it to be neglected relative to $t\bar{t}$ +jets and enabling a uniform event categorization strategy across all three channels, as depicted in Fig. 5 in the End Matter. Only events with a high $t\bar{t}H$ or $t\bar{t}Z$ likelihood—defined as $\mathcal{D}_{t\bar{t}X} > 0.6$, where $\mathcal{D}_{t\bar{t}X}$ is the sum of all four $t\bar{t}H$ and $t\bar{t}Z$ discriminants—are retained for signal extraction and background estimation. A selection on the $t\bar{t}$ +light discriminant further reduces $t\bar{t}$ +light contamination. Events passing these criteria are categorized into four signal regions (SRs) with $\mathcal{D}_{t\bar{t}X} > 0.85$, each enriched in $t\bar{t}H(H \rightarrow c\bar{c})$, $t\bar{t}H(H \rightarrow b\bar{b})$, $t\bar{t}Z(Z \rightarrow c\bar{c})$, and $t\bar{t}Z(Z \rightarrow b\bar{b})$, along with five control regions (CRs) with $0.6 < \mathcal{D}_{t\bar{t}X} < 0.85$, which are used to estimate the normalizations of various $t\bar{t}$ +jets background components in a phase space similar to that of the SRs. Additional requirements on heavy-flavor jet multiplicity enhance purity: at least three b jets are required for the b -enriched regions ($t\bar{t}H(H \rightarrow b\bar{b})$, $t\bar{t}Z(Z \rightarrow b\bar{b})$, $t\bar{t}+\geq 2b$, and $t\bar{t}+b$), while at least two (or one) c jets are required for the c -enriched $t\bar{t}H(H \rightarrow c\bar{c})$, $t\bar{t}Z(Z \rightarrow c\bar{c})$, and $t\bar{t}+\geq 2c$ ($t\bar{t}+c$) regions. A signal-depleted sideband region, defined by $0.4 < \mathcal{D}_{t\bar{t}X} < 0.6$ with an analogous SR and CR structure, is used to validate the background estimation strategy.

Production rates of the signal processes are determined via a binned profile likelihood fit to data. The fitted variable is the PART classifier discriminant for each category. For each of the $t\bar{t}H(H \rightarrow c\bar{c})$, $t\bar{t}H(H \rightarrow b\bar{b})$, $t\bar{t}Z(Z \rightarrow c\bar{c})$, and $t\bar{t}Z(Z \rightarrow b\bar{b})$ processes, the expected yield is scaled by an independent signal strength modifier μ , defined as $(\sigma\mathcal{B})_{\text{obs}}/(\sigma\mathcal{B})_{\text{SM}}$. Here σ is the production cross section and $\mathcal{B}$ is the branching fraction, which is allowed to freely float in the fit, following the procedure in Ref. [17]. The dominant background, $t\bar{t}$ +jets, is estimated by including CRs in the fit, with the normalizations of the $t\bar{t}+c$, $t\bar{t}+\geq 2c$, $t\bar{t}+b$, $t\bar{t}+\geq 2b$, and $t\bar{t}$ +light components allowed to float independently. The normalization factors for each $t\bar{t}$ +jets component are shared between the 1L and 2L channels but not with the 0L channel, to account for potential phase space differences due to the requirement of more energetic jets in the 0L case. Minor backgrounds, such as single top quark production, $t\bar{t}W$, and tWZ , are estimated directly from simulations assuming SM production rates. Results are obtained using COMBINE [76], the CMS statistical analysis tool based on the ROOFIT [77] and ROOSTATS [78] frameworks.

Systematic uncertainties affecting normalizations and shapes of fitted variables are incorporated via nuisance parameters. The contributions of each uncertainty source to the total uncertainty in the fitted $\mu_{t\bar{t}H(H \rightarrow c\bar{c})}$ and $\mu_{t\bar{t}H(H \rightarrow b\bar{b})}$ are summarized in Table 2 in the End Matter. For $\mu_{t\bar{t}H(H \rightarrow c\bar{c})}$, the leading uncertainty is statistical because of the limited number of events in the SRs as well as in the CRs used to extract background normalizations. The main systematic uncertainty arises from the theoretical modeling of the $t\bar{t}+c$ and $t\bar{t}$ +light processes, contributing $\approx 32\%$ and $\approx 29\%$ of the total uncertainty, respectively. For $\mu_{t\bar{t}H(H \rightarrow b\bar{b})}$, the largest uncertainties are theoretical, including those associated with the renormalization and factorization scales, flavor scheme, and parton shower modeling in the $t\bar{t}b\bar{b}$ simulation, representing $\approx 60\%$ of the

total uncertainty. Theoretical uncertainties in the $t\bar{t}H$ signal simulation contribute an additional $\approx 47\%$. For both measurements, the primary experimental uncertainty is associated with jet flavor identification efficiencies, representing $\approx 39\%$ ($\approx 28\%$) of the total uncertainty in $\mu_{t\bar{t}H(H \rightarrow c\bar{c})}$ ($\mu_{t\bar{t}H(H \rightarrow b\bar{b})}$).

The analysis is validated by measuring the $t\bar{t}Z$ signal strengths:

$$\begin{aligned}\mu_{t\bar{t}Z(Z \rightarrow c\bar{c})} &= 1.02^{+0.79}_{-0.84}, \\ \mu_{t\bar{t}Z(Z \rightarrow b\bar{b})} &= 1.47^{+0.45}_{-0.41},\end{aligned}\tag{1}$$

which are consistent with the SM prediction within uncertainties and with measurements in the leptonic decay channel [79–81]. The significance of the excess over the background-only hypothesis is computed using the asymptotic distribution of a test statistic based on the profile likelihood ratio [82, 83]. The observed (expected) significance is 1.2 (1.3) standard deviations for $t\bar{t}Z(Z \rightarrow c\bar{c})$ and 3.5 (2.4) standard deviations for $t\bar{t}Z(Z \rightarrow b\bar{b})$.

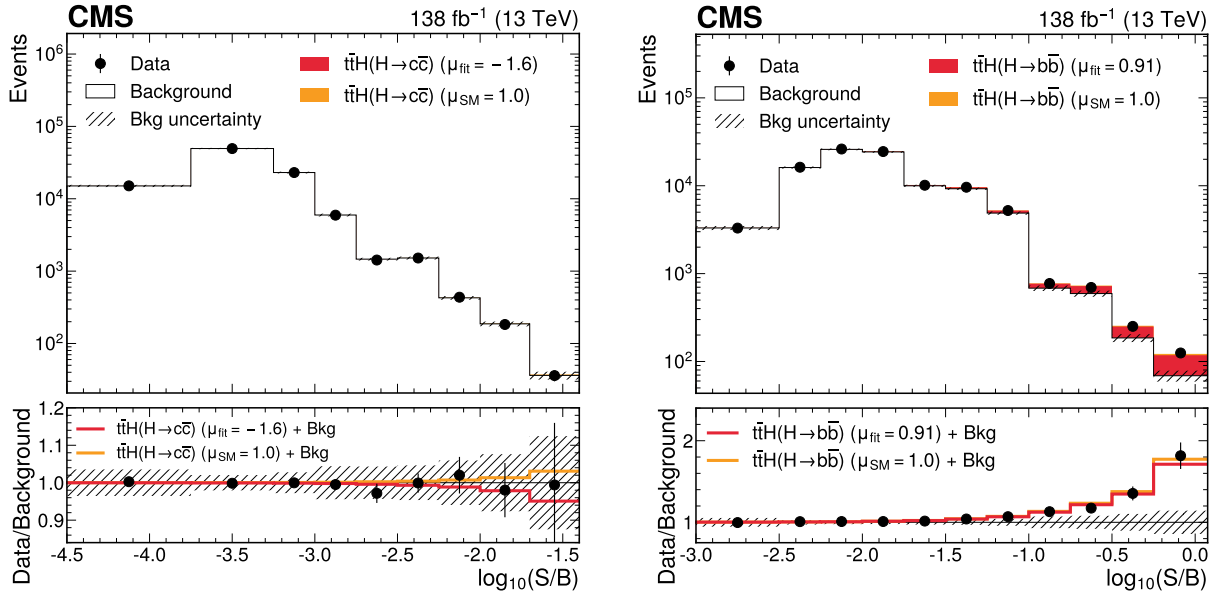


Figure 2: Observed and expected event yields from all SRs and CRs as a function of $\log_{10}(S/B)$, where S are the expected $t\bar{t}H(H \rightarrow c\bar{c})$ (left) and $t\bar{t}H(H \rightarrow b\bar{b})$ (right) yields, and B are the post-fit total background yields. Signal contributions are shown for the best fit signal strength (red) and for the SM prediction, $\mu = 1$ (orange). The lower panel shows the ratio of the data to the post-fit background predictions, compared to the signal-plus-background predictions.

Figure 2 shows the observed and expected event yields from all CRs and SRs as a function of $\log_{10}(S/B)$, the logarithm of the ratio of $t\bar{t}H(H \rightarrow c\bar{c})$ (or $t\bar{t}H(H \rightarrow b\bar{b})$) and background yields. The best fit signal strengths for $t\bar{t}H$ production are

$$\begin{aligned}\mu_{t\bar{t}H(H \rightarrow c\bar{c})} &= -1.6 \pm 4.5, \\ \mu_{t\bar{t}H(H \rightarrow b\bar{b})} &= 0.91^{+0.26}_{-0.22},\end{aligned}\tag{2}$$

with an observed (expected) significance of 4.4 (4.5) standard deviations for the $t\bar{t}H(H \rightarrow b\bar{b})$ process. The best fit $\mu_{t\bar{t}H(H \rightarrow b\bar{b})}$ value is closer to the SM prediction than was the previous measurement [84], with a compatibility p -value of 10% (3%) between the two measurements, assuming uncorrelated (50% correlated) systematic uncertainties. Because of a very different

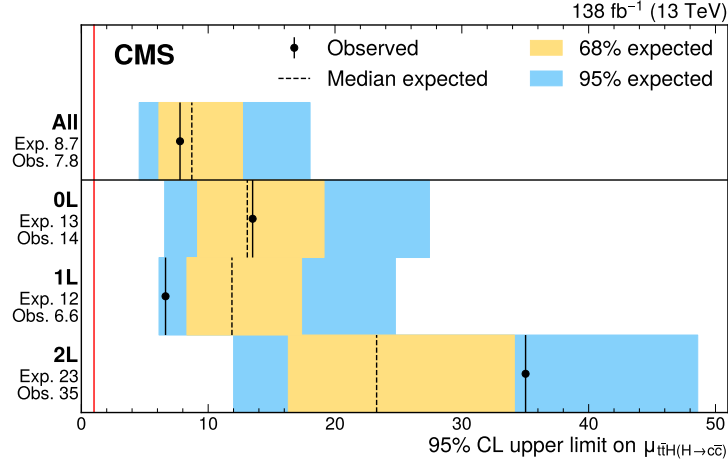


Figure 3: The 95% CL upper limits on $\mu_{t\bar{t}H(H\rightarrow c\bar{c})}$. The yellow and blue bands indicate the expected 68% and 95% CL regions, respectively, under the background-only hypothesis. The vertical red line indicates the SM value $\mu_{t\bar{t}H(H\rightarrow c\bar{c})} = 1$.

background model, a more inclusive event selection, and a low correlation of the neural network scores, the total systematic uncertainty can be considered mostly uncorrelated. No excess over the background-only hypothesis is observed in the search for $t\bar{t}H(H\rightarrow c\bar{c})$. An upper limit on $\mu_{t\bar{t}H(H\rightarrow c\bar{c})}$ is extracted using the CL_s criterion [85, 86]. The test statistic is the profile likelihood ratio modified for upper limits [82], with the asymptotic approximation [83] used in the limit setting procedure. The observed (expected) 95% CL upper limit on $\mu_{t\bar{t}H(H\rightarrow c\bar{c})}$ is $7.8 (8.7^{+4.0}_{-2.6})$, corresponding to an observed (expected) upper limit on $\sigma(t\bar{t}H)\mathcal{B}(H\rightarrow c\bar{c})$ of $0.11 (0.13^{+0.06}_{-0.04})$ pb. The contributions from the individual channels are summarized in Fig. 3. Tabulated results are provided in the HEPData record for this analysis [87].

The result is interpreted in the κ -framework [88, 89] by reparameterizing $\mathcal{B}(H\rightarrow c\bar{c})$ and $\mathcal{B}(H\rightarrow b\bar{b})$ in terms of the charm and bottom quark Yukawa coupling modifiers κ_c and κ_b , assuming that only the Higgs boson decay widths are altered:

$$\begin{aligned}\mathcal{B}(H\rightarrow c\bar{c}) &= \frac{\kappa_c^2 \mathcal{B}_{SM}^{H\rightarrow c\bar{c}}}{1 + (\kappa_c^2 - 1) \mathcal{B}_{SM}^{H\rightarrow c\bar{c}} + (\kappa_b^2 - 1) \mathcal{B}_{SM}^{H\rightarrow b\bar{b}}}, \\ \mathcal{B}(H\rightarrow b\bar{b}) &= \frac{\kappa_b^2 \mathcal{B}_{SM}^{H\rightarrow b\bar{b}}}{1 + (\kappa_c^2 - 1) \mathcal{B}_{SM}^{H\rightarrow c\bar{c}} + (\kappa_b^2 - 1) \mathcal{B}_{SM}^{H\rightarrow b\bar{b}}}.\end{aligned}\tag{3}$$

Figure 4 shows the two-dimensional profile likelihood scan of κ_c and κ_b . When fixing κ_b to the SM expectation, the observed (expected) 95% CL interval is $|\kappa_c| < 3.0 (3.3)$.

A combined analysis with the previous search in the VH channel [27] is performed. Common experimental uncertainties are correlated, except for jet flavor tagging, which differs in algorithms and calibration methods. Background modeling uncertainties are uncorrelated because of differing dominant backgrounds, while theoretical uncertainties in Higgs boson production and decay for the same processes are correlated. The observed (expected) 95% CL upper limit on $\mu_{H\rightarrow c\bar{c}}$, assuming SM production rates for $t\bar{t}H$ and VH, is $9.3 (5.6^{+2.4}_{-1.6})$. For κ_c , the combination improves the expected 95% CL interval to $|\kappa_c| < 2.7$, while the observed is $|\kappa_c| < 3.5$.

In summary, a search for the SM Higgs boson decaying to a charm quark-antiquark pair via $t\bar{t}H$ production is presented, alongside a simultaneous measurement of the Higgs boson de-

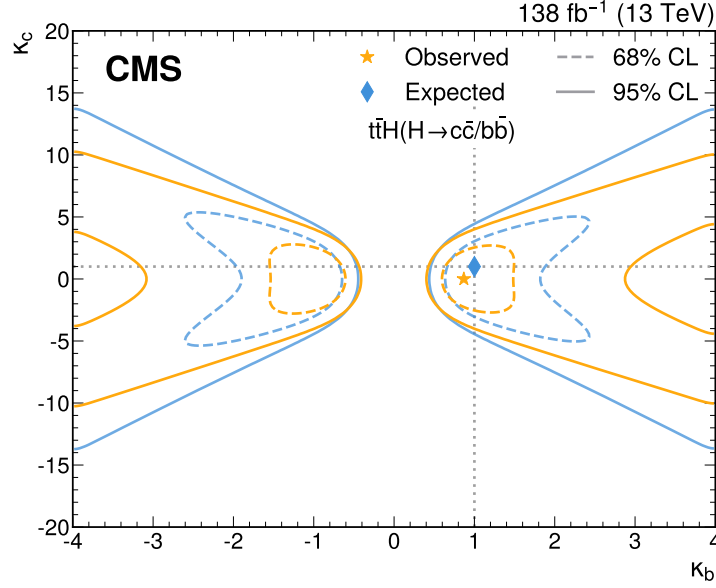


Figure 4: Constraints on the Higgs boson coupling modifiers κ_c and κ_b . The 68% (95%) CL intervals are indicated by the dashed (solid) lines. The observed (expected) best fit values are shown by the orange (blue) markers.

cay to a bottom quark-antiquark pair. Novel jet flavor identification tools and event classification techniques using advanced machine learning algorithms are developed for this analysis. The observed $t\bar{t}H$ signals relative to the SM predictions are $\mu_{t\bar{t}H(H \rightarrow c\bar{c})} = -1.6 \pm 4.5$ and $\mu_{t\bar{t}H(H \rightarrow b\bar{b})} = 0.91^{+0.26}_{-0.22}$, with an observed (expected) significance of 4.4 (4.5) standard deviations for the $t\bar{t}H(H \rightarrow b\bar{b})$ process. The observed (expected) upper limit on $\sigma(t\bar{t}H)\mathcal{B}(H \rightarrow c\bar{c})$ is 0.11 ($0.13^{+0.06}_{-0.04}$) pb, corresponding to 7.8 ($8.7^{+4.0}_{-2.6}$) times the theoretical prediction for an SM Higgs boson mass of 125.38 GeV. When combined with the previous search for $H \rightarrow c\bar{c}$ via associated production with a W or Z boson, the observed (expected) 95% CL interval on the charm quark Yukawa coupling modifier, κ_c , is $|\kappa_c| < 3.5$ (2.7). This represents the most stringent constraint on κ_c to date.

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A End Matter

A.1 Analysis strategy and event selection

The PART event classifier is used to select and categorize events, as illustrated in Fig. 5. The classifier outputs 10 (9) likelihood scores that sum to unity for the 0L (1L and 2L) channel. These include four scores for the signal processes, $\mathcal{D}_{t\bar{t}H(H \rightarrow c\bar{c})}$, $\mathcal{D}_{t\bar{t}H(H \rightarrow b\bar{b})}$, $\mathcal{D}_{t\bar{t}Z(Z \rightarrow c\bar{c})}$, and $\mathcal{D}_{t\bar{t}Z(Z \rightarrow b\bar{b})}$, and six (five) for the background processes, $\mathcal{D}_{t\bar{t}+\text{light}}$, $\mathcal{D}_{t\bar{t}+c}$, $\mathcal{D}_{t\bar{t}+\geq 2c}$, $\mathcal{D}_{t\bar{t}+b}$, $\mathcal{D}_{t\bar{t}+\geq 2b}$, and $\mathcal{D}_{QCD}$ (the last applies only to the 0L channel). The sum of the four signal scores is defined as $\mathcal{D}_{t\bar{t}X}$, while the sum of the five $t\bar{t}$ +jets background scores is defined as $\mathcal{D}_{t\bar{t}+\text{jets}}$.

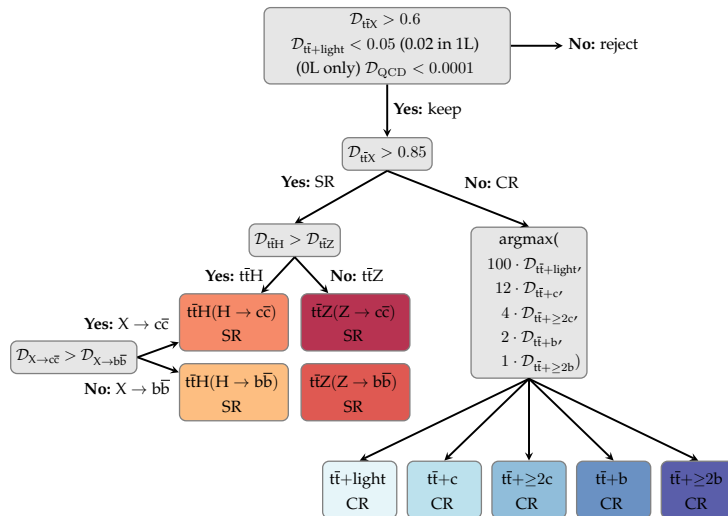


Figure 5: Event categorization flowchart.

In the 0L channel, an initial requirement of $\mathcal{D}_{QCD} < 0.0001$ suppresses the QCD multijet background to below 1% of the $t\bar{t}$ +jets background, allowing the QCD multijet contribution to be neglected. To reduce the $t\bar{t}$ +light background, a requirement of $\mathcal{D}_{t\bar{t}+light} < 0.05$ (0.02) is applied in the 0L and 2L (1L) channels. Events with $\mathcal{D}_{t\bar{t}X} > 0.85$ are assigned to one of four SRs based on two pairs of signal discriminants, $\mathcal{D}_{t\bar{t}H}$ vs. $\mathcal{D}_{t\bar{t}Z}$ and $\mathcal{D}_{X \rightarrow c\bar{c}}$ vs. $\mathcal{D}_{X \rightarrow b\bar{b}}$, where $\mathcal{D}_{t\bar{t}H} = \mathcal{D}_{t\bar{t}H(H \rightarrow c\bar{c})} + \mathcal{D}_{t\bar{t}H(H \rightarrow b\bar{b})}$, $\mathcal{D}_{t\bar{t}Z} = \mathcal{D}_{t\bar{t}Z(Z \rightarrow c\bar{c})} + \mathcal{D}_{t\bar{t}Z(Z \rightarrow b\bar{b})}$, $\mathcal{D}_{X \rightarrow c\bar{c}} = \mathcal{D}_{t\bar{t}H(H \rightarrow c\bar{c})} + \mathcal{D}_{t\bar{t}Z(Z \rightarrow c\bar{c})}$, and $\mathcal{D}_{X \rightarrow b\bar{b}} = \mathcal{D}_{t\bar{t}H(H \rightarrow b\bar{b})} + \mathcal{D}_{t\bar{t}Z(Z \rightarrow b\bar{b})}$. Events with $0.6 < \mathcal{D}_{t\bar{t}X} < 0.85$ are categorized into one of the five CRs, determined by the background class with the highest weighted score. The weights—100, 12, 4, 2 and 1 for $\mathcal{D}_{t\bar{t}+light}$, $\mathcal{D}_{t\bar{t}+c}$, $\mathcal{D}_{t\bar{t}+\geq 2c}$, $\mathcal{D}_{t\bar{t}+b}$, $\mathcal{D}_{t\bar{t}+\geq 2b}$, respectively—are optimized to enhance the purity of each CR.

Figure 6 shows the fitted event yields in each bin for the CRs and SRs.

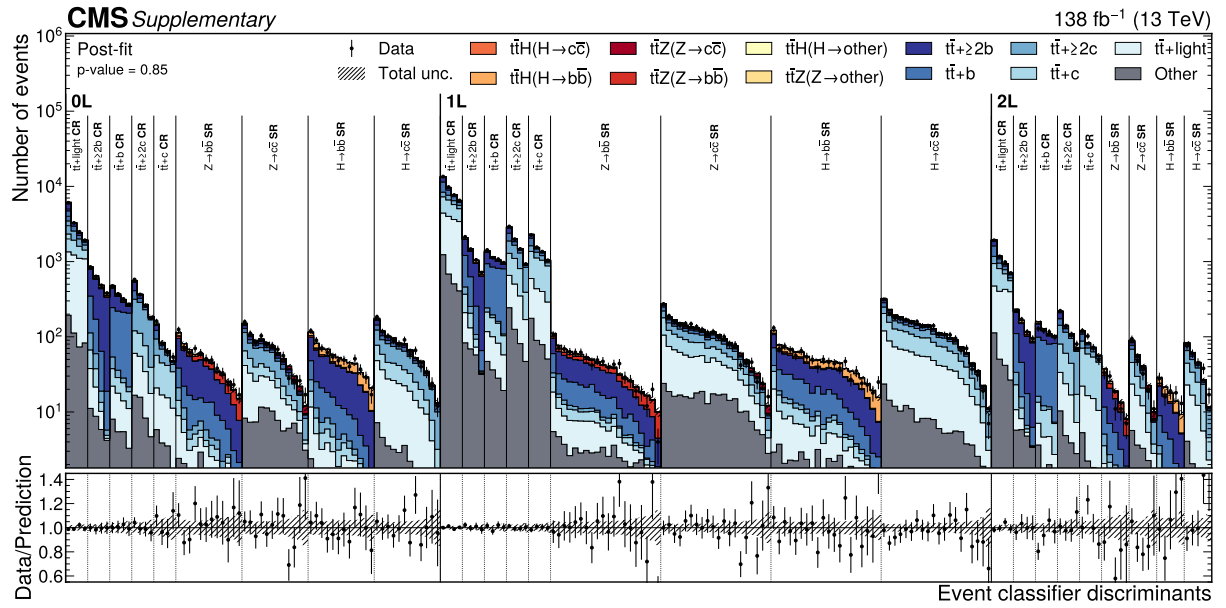


Figure 6: Distributions of the PART discriminants in data (points) and predicted signal and backgrounds (colored histograms) after the fit to data. The vertical bars on the points represent the statistical uncertainties in data. The hatched band represents the total uncertainty in the sum of the signal and background predictions. The lower panel shows the ratio of the data to the sum of the signal and background predictions.

A.2 The $t\bar{t}$ +jets background model

Simulated $t\bar{t}$ +jets events are divided into five mutually exclusive components: $t\bar{t}+\geq 2b$, $t\bar{t}+b$, $t\bar{t}+\geq 2c$, $t\bar{t}+c$, and $t\bar{t}+light$. The $t\bar{t}+\geq 2b$ and $t\bar{t}+b$ events are taken from a dedicated $t\bar{t}b\bar{b}$ sample, where the $t\bar{t}b\bar{b}$ matrix elements are calculated at NLO in QCD using the four-flavor scheme (4FS). The b quark mass is set to 4.75 GeV, and the 4FS NNLO NNPDF3.1 PDF set is used to describe the proton structure. The $t\bar{t}b\bar{b}$ production cross section is computed at NLO in 4FS. The $t\bar{t}+\geq 2c$, $t\bar{t}+c$, and $t\bar{t}+light$ components are extracted from the inclusive $t\bar{t}$ simulation after removing the $t\bar{t}+\geq 2b$ and $t\bar{t}+b$ contributions, thereby avoiding double counting. This inclusive $t\bar{t}$ sample is generated at NLO in QCD with up to one additional parton included at the matrix-element level, while additional emissions are modeled via parton showering with PYTHIA. The matrix element calculation is performed in the five-flavor scheme (5FS) using the 5FS NNLO NNPDF3.1 PDF set, where the b quarks are treated as massless. A subcomponent of $t\bar{t}+b$ ($t\bar{t}+c$), referred to as $t\bar{t}+j_{bb}$ ($t\bar{t}+j_{cc}$), consists of events where the additional b (c) jet

contains two or more b (c) hadrons. These events predominantly arise from collinear $g \rightarrow b\bar{b}$ ($g \rightarrow c\bar{c}$) splittings, which are not well modeled in simulation. To account for this modeling limitation, an additional 50% uncertainty is assigned to the $t\bar{t}+j_{bb}$ and $t\bar{t}+j_{cc}$ contributions in the background estimation.

Production of $t\bar{t}b\bar{b}$ via double parton scattering (DPS) also contributes to the $t\bar{t}+\geq 2b$ and $t\bar{t}+b$ categories. This contribution is included in the inclusive $t\bar{t}$ sample but not in the dedicated $t\bar{t}b\bar{b}$ sample. It is therefore modeled separately by generating $t\bar{t}$ production at NLO in QCD using POWHEG, with additional $b\bar{b}$ production simulated by PYTHIA at LO in QCD using the *SecondHard* option. The cross section for this process is estimated to be 8 pb, assuming an effective DPS cross section of 30 mb [90] and an inclusive $b\bar{b}$ cross section of 0.3 mb, the latter estimated from simulation. In the background estimation, the DPS contributions are included in the corresponding $t\bar{t}+\geq 2b$ and $t\bar{t}+b$ categories, with a 50% uncertainty assigned to the normalization of the DPS components.

Table 1 summarizes the best fit values of the $t\bar{t}+\text{jets}$ background normalization factors obtained from a simultaneous fit to all CRs and SRs.

Table 1: Best fit values of the $t\bar{t}+\text{jets}$ background normalization factors for each analysis category (Cat.).

Cat.	$t\bar{t}+\geq 2b$	$t\bar{t}+b$	$t\bar{t}+\geq 2c$	$t\bar{t}+c$	$t\bar{t}+\text{light}$
2L/1L	0.88 ± 0.07	0.92 ± 0.16	1.39 ± 0.23	1.41 ± 0.36	0.89 ± 0.11
0L	1.12 ± 0.11	0.89 ± 0.18	2.03 ± 0.41	0.95 ± 0.34	0.89 ± 0.17

A.3 Uncertainty breakdown

Table 2: The absolute (relative) contributions to the total uncertainties, $\Delta\mu$ ($\Delta\mu/\Delta\mu_{\text{tot}}$).

Uncertainty source	$\Delta\mu$ ($\Delta\mu/\Delta\mu_{\text{tot}}$)	
	$\mu_{t\bar{t}H(H \rightarrow c\bar{c})}$	$\mu_{t\bar{t}H(H \rightarrow b\bar{b})}$
Statistical	3.3 (74%)	0.14 (57%)
$t\bar{t}+\text{jets}$ normalizations	1.4 (32%)	0.06 (26%)
$t\bar{t}Z$ normalizations	0.4 (8.4%)	0.06 (30%)
Theory	2.1 (47%)	0.18 (75%)
Signal	0.7 (15%)	0.11 (47%)
$t\bar{t}+\geq 1b$	0.7 (15%)	0.14 (60%)
$t\bar{t}+\geq 1c$	1.4 (32%)	0.01 (5.8%)
$t\bar{t}+\text{light}$	1.3 (29%)	0.01 (5.2%)
Minor backgrounds	0.2 (4.6%)	0.01 (4.6%)
Experimental	2.0 (47%)	0.07 (31%)
Jet flavor tagging	1.7 (39%)	0.07 (28%)
Size of the simulated samples	1.1 (24%)	0.05 (21%)
Jet energy scale and resolution	0.8 (18%)	0.02 (8.6%)
Lepton identification	0.3 (6.0%)	0.02 (6.3%)
Integrated luminosity	0.1 (2.0%)	0.02 (6.2%)
Total	4.5 (100%)	0.24 (100%)

The contributions of individual uncertainty sources to the total uncertainties in the fitted $\mu_{t\bar{t}H(H \rightarrow c\bar{c})}$ and $\mu_{t\bar{t}H(H \rightarrow b\bar{b})}$ are summarized in Table 2. The values are determined by repeat-

ing the fit with the nuisance parameters associated with each category fixed to their best fit values, and then subtracting the resulting uncertainty in quadrature from the total uncertainty. The total uncertainty differs from the quadrature sum of the individual components because of correlations among nuisance parameters in the fit.

B Supplemental Material

B.1 Simulated samples

Signal and background processes are modeled using Monte Carlo (MC) simulations. The generators used for the $t\bar{t}H$, $t\bar{t}Z$, and $t\bar{t}$ processes are listed in Table B.1, while those for the other background processes are summarized in Table B.2. The decays of heavy particles in $t\bar{t}W$, $t\bar{t}Z$, and t -channel single top quark production are modeled using MADSPIN [91]. Details about the modeling parameters of the $t\bar{t}b\bar{b}$ sample in the four-flavor scheme (4FS) and of the inclusive $t\bar{t}$ sample in the five-flavor scheme (5FS) are provided in Table B.3.

The QCD multijet events are generated with MADGRAPH5_aMC@NLO at leading-order (LO) accuracy, employing the MLM scheme [68] for matrix element (ME) and parton shower (PS) matching, and are used only for training the neural network event classifier and are not included in the background estimation for the profile likelihood fits.

Table B.1: Generator settings for signal and major background samples. The “Groups” column refers to the grouping of processes in the maximum likelihood fits. Here, $t\bar{t}H(H \rightarrow \text{Other})$ and $t\bar{t}Z(Z \rightarrow \text{Other})$ refer to all Higgs boson and Z boson decay channels other than those to b and c quark pairs.

Process	Groups	ME order	Generator	Notes
$t\bar{t}H$	$t\bar{t}H(H \rightarrow c\bar{c}), t\bar{t}H(H \rightarrow b\bar{b}), t\bar{t}H(H \rightarrow \text{Other})$	NLO	POWHEG v2	
$t\bar{t}Z$	$t\bar{t}Z(Z \rightarrow c\bar{c}), t\bar{t}Z(Z \rightarrow b\bar{b}), t\bar{t}Z(Z \rightarrow \text{Other})$	NLO	MADGRAPH5_aMC@NLO v2.6.1	MADSPIN for heavy particle decays
$t\bar{t}$	$t\bar{t} + \text{light}, t\bar{t} + \geq 2c, t\bar{t} + c$	NLO	POWHEG v2	
$t\bar{t}b\bar{b}$	$t\bar{t} + \geq 2b, t\bar{t} + b$	NLO	POWHEG-BOX-RES	
$t\bar{t}b\bar{b}$ DPS	$t\bar{t} + \geq 2b, t\bar{t} + b$	NLO / LO	POWHEG v2 / PYTHIA v8.240	$t\bar{t}$ NLO ME with POWHEG / LO $b\bar{b}$ DPS with PYTHIA

Table B.2: Generator settings for minor background samples. The “Group” column refers to the grouping of processes in the maximum likelihood fits.

Process	Group	ME order	Generator	Notes
tW			POWHEG v2	
t channel s channel	single t	NLO	POWHEG v2 MADGRAPH5_aMC@NLO v2.6.1	MADSPIN for heavy particle decays
$t\bar{t}W$	$t\bar{t}W$	NLO	MADGRAPH5_aMC@NLO v2.6.1	FxFx merging up to 1 additional jet MADSPIN for heavy particle decays
tWZ	tWZ	LO	MADGRAPH5_aMC@NLO v2.6.5	MADSPIN for heavy particle decays
QCD	QCD	LO	MADGRAPH5_aMC@NLO v2.5.1	MLM merging for ME-PS matching

B.2 Jet flavor identification

Jets containing b or c hadrons are identified using the PARTICLENET algorithm [33]. The PARTICLENET algorithm outputs eight probabilities, trained to discriminate jets containing one (p_b) or two (p_{bb}) b hadrons, one (p_c) or two (p_{cc}) c hadrons, jets originating from u, d, or s quarks (p_{uds}), gluons (p_g), pileup, or other sources. For this measurement, it is essential to distinguish jets originating from b quarks, c quarks, and those of other origins. Therefore, two discrimi-

Table B.3: Summary of generator settings used for the $t\bar{t}b\bar{b}$ and inclusive $t\bar{t}$ samples. The transverse mass is defined as $m_T = \sqrt{m^2 + p_T^2}$.

	$t\bar{t}$ NLO (5FS)	$t\bar{t}b\bar{b}$ NLO (4FS)
ME generator	POWHEG v2	POWHEG-BOX-RES
Parton shower	PYTHIA v8.230	PYTHIA v8.230
Flavor scheme	5FS	4FS
PDF set	NNPDF31_nnlo_hessian_pdfas	NNPDF31_nnlo_as_0118_nf_4
m_t	172.5 GeV	172.5 GeV
m_b	0	4.75 GeV
μ_R	$\sqrt{\frac{1}{2}(m_{rT,t}^2 + m_{T,\bar{t}}^2)}$	$\frac{1}{2} \sqrt[4]{m_{t,t} m_{t,\bar{t}} m_{t,b} m_{t,\bar{b}}}$
μ_F	μ_R	$\frac{1}{4} [m_{t,t} + m_{t,\bar{t}} + m_{t,b} + m_{t,\bar{b}} + m_{t,g}]$
h_{damp}	$1.379 m_t$	$1.379 m_t$
Tune	CP5	CP5

nants are constructed, based on the individual output probabilities of the PARTICLENET tagger:

$$\begin{aligned}
 p_{B+C} &= \frac{p_b + p_{bb} + p_c + p_{cc}}{p_b + p_{bb} + p_c + p_{cc} + p_{uds} + p_g}, \\
 p_{BvsC} &= \frac{p_b + p_{bb}}{p_b + p_{bb} + p_c + p_{cc}}.
 \end{aligned} \tag{4}$$

The first discriminant, p_{B+C} , differentiates between heavy-flavor (HF) jets (i.e., of b or c origin) and light jets (i.e., of u, d, s, and g origin). The second discriminant, p_{BvsC} , further separates HF jets into b and c jets. Based on these two discriminants, 11 mutually exclusive tagging categories are defined: 5 categories for b tagging (B0–B4), 5 categories for c tagging (C0–C4), and one untagged category (L0).

In Fig. B.1, the rejection factors, i.e., the inverse of the efficiency, for the subdominant jet flavors in each of the categories are compared to the DEEPIET tagger [75] used in previous $H \rightarrow c\bar{c}$ searches. For this purpose, similar working points were derived for the DEEPIET tagger, mimicking the tagging efficiencies of the dominant jet flavor in each of the tagging bins, i.e., requiring the same light-jet efficiency in L0, the same c jet efficiency in C0–C4, and the same b jet efficiency in B1–B4. The bin B0 is not shown as no comparable b tagging efficiency for DEEPIET can be achieved for all bins at the same time due to its lower overall tagging efficiency. In summary, the tagging layout of the PARTICLENET algorithm improves the rejection factors of the subdominant jet flavors by factors of 1–2 in all tagging bins, compared to DEEPIET.

Differences in the flavor tagging efficiencies between simulation and data are measured using three data samples, enriched each in dileptonic $t\bar{t}$, W+jets, and Z+jets events, focusing on b, c, and light jets, respectively.

- The $t\bar{t}$ region is defined by selecting events that contain an $e \pm \mu \mp$ pair. In addition, the transverse mass $m_T(e, \mu, p_T^{\text{miss}})$ is required to be larger than 100 GeV to reduce contributions of Z+jets events.
- For the W+jets region, events with one isolated lepton are selected. Events further need to have exactly one jet that contains a nonisolated muon with a p_T larger than 5 GeV inside the jet cone and with a charge opposite to that of the selected isolated lepton. The requirement of a non-isolated muon inside the jet cone enriches the selection in events with semileptonic c hadron decays in the jets, and thereby W+c

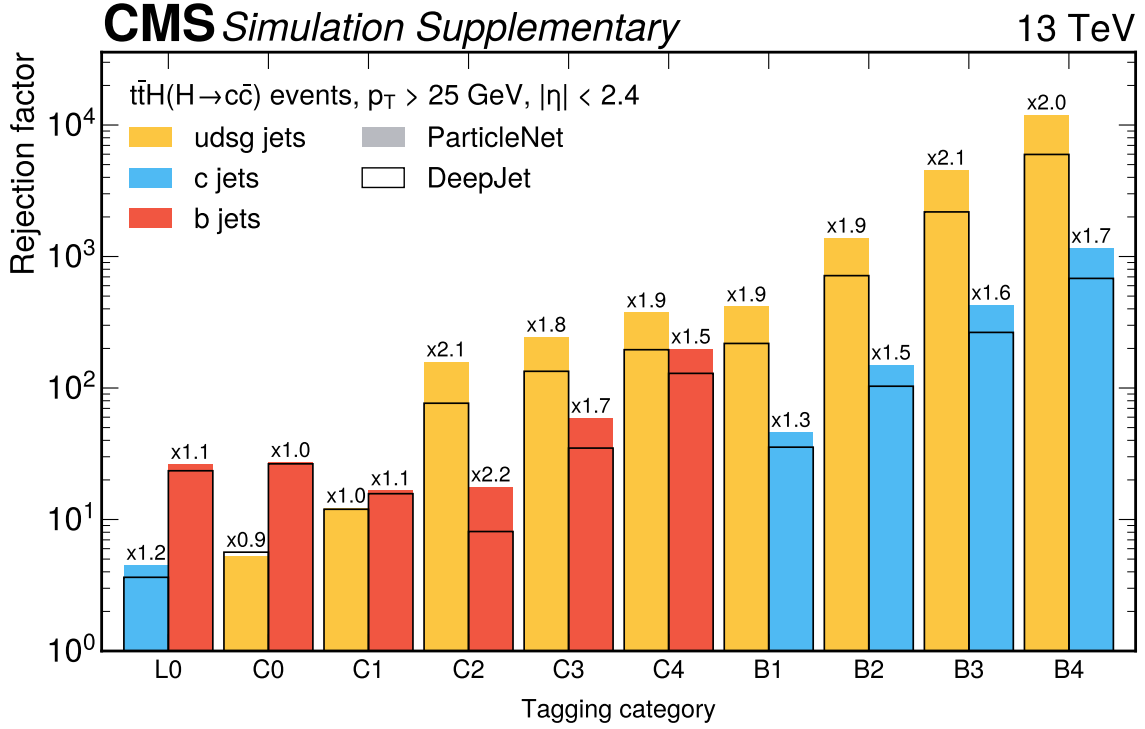


Figure B.1: Rejection factors for the subdominant jet flavors in each of the tagging bins. The filled bars represent the rejection factors achieved with the PARTICLENET tagger and the corresponding working point definitions. The black bars represent the rejection factors achieved with the DEEPIJET tagger with working points mimicking the dominant flavor tagging efficiencies. Each bin is labeled with the relative improvement of the PARTICLENET tagger compared to the DEEPIJET tagger. All rejection factors and tagging efficiencies are evaluated using simulated $t\bar{t}H(H \rightarrow c\bar{c})$ events with 2018 detector conditions.

signatures. A set of additional kinematic requirements are imposed to reduce contributions from other background processes and enrich the selection with W +jets events.

- Finally, for the Z +jets region, events with two opposite-charge same-flavor (e^+e^- , $\mu^+\mu^-$) lepton candidates are selected. The leading lepton is required to have $p_T > 25$ GeV, and $m_{\ell\ell}$ has to be within the range of 81–101 GeV. Exactly one additional jet in the event that balances the reconstructed Z boson p_T is required.

For all regions, the jets are selected using the same criteria as used in the present $t\bar{t}H(H \rightarrow c\bar{c})$ analysis.

Simulation-to-data scale factors (SFs) are then derived as a function of jet p_T with the following procedure. Tagging SFs are derived by simultaneously fitting all three flavor-enriched regions (Z +jets, W +jets, $t\bar{t}$) in a profile likelihood fit. The tagging SFs are discretized into the eleven aforementioned tagging bins L0, C0–C4, and B0–B4. For each of the ten exclusive C0–C4 and B0–B4 bins, one parameter of interest (POI) is defined per jet flavor (i.e., in total 30 independent POIs per jet p_T bin), which corresponds to the jet tagging scale factor for the exclusive tagging bin and jet flavor. In order to preserve unitarity, the SFs for the tagger bin L0 are not associated with an independent POI but are constructed such that the sum of tagging probabilities per jet

flavor is retained, i.e., requiring

$$\sum_{\text{WP} \in [\text{L0}, \text{C0} - \text{C4}, \text{B0} - \text{B4}]} \epsilon_{\text{MC}}(\text{WP}|\text{flav}) = \sum_{\text{WP}} \epsilon_{\text{data}}(\text{WP}|\text{flav}) \equiv 1. \quad (5)$$

This constraint guarantees that the overall normalization of each type (b, c, and light) component is retained in the fits, and the resulting SFs correct for only the efficiencies but do not alter the normalizations. This helps preserve the normalization of each flavor component when the SFs are applied to a different phase space region. To be insensitive to the overall normalization of the total background prediction as obtained by the simulation and to fit only the relative tagging efficiencies, the overall expected yields are scaled to match the observed data in the scale factor derivation regions, inclusive in jet flavor. The fits are performed in six independent jet p_T ranges, to introduce a p_T dependence on the tagging SFs:

$$p_T(\text{jet}) \in [25, 35, 50, 70, 90, 120, \infty] \text{ GeV}. \quad (6)$$

The normalization and derivation of SFs is completely independent for each of the p_T ranges.

In some cases, where the contribution of a certain jet flavor to a certain tagging bin is very small, the SFs cannot be determined well. For example, in the high b tagging bins B3 or B4, the contamination of c and LF jets is almost negligible. In cases where the fits for these parameters do not lead to a well-converged result, i.e., where the expected uncertainty in the SF exceeds 50%, the SF value is set to unity in the fit to data, and the corresponding SF is assigned an uncertainty covering the range $[0.3, 3]$. Changes in these SFs have negligible impact on the analysis results, as the contamination of jets of the affected flavors in the corresponding tagging bins is negligible.

In the fit to data, a range of experimental and modeling uncertainties are considered. The same set of experimental uncertainties as described in Section B.6 is considered for the calibration measurement. Modeling uncertainties due to renormalization scale μ_R and factorization scale μ_F choices, and uncertainties due to initial-state and final-state radiation scales (ISR and FSR) are applied, following the same procedures as described in Section B.7. These uncertainties are treated as uncorrelated between major processes in the SF derivation regions ($t\bar{t}$, W +jets, Z +jets, etc.). Normalization uncertainties are included to account for the limited knowledge of the cross sections of the relevant processes. A 5% normalization uncertainty is applied to the minor $t\bar{t}$ background in the W +jets and Z +jets regions. In the $t\bar{t}$ channel, the $t\bar{t}$ normalization is fitted to data. A 10% normalization uncertainty is applied for tW production, and 15% for single top t -channel production. Diboson production is associated with a 15% normalization uncertainty. For the production of a W or Z boson with HF jets, dedicated normalization uncertainties are applied, as the modeling of these processes is known to be insufficient. An 8% normalization uncertainty is applied to W +c production. The W +b, Z +b, and Z +c processes are each associated with a free parameter in the fit to determine the normalization in-situ.

The impacts of systematic uncertainties in the final tagging SFs are derived from the impacts of the corresponding nuisance parameters. Variations of a systematic source are considered fully correlated between all SFs, p_T ranges, and years when applied in the $t\bar{t}H(H \rightarrow c\bar{c})$ analysis. The statistical uncertainties are derived by freezing all nuisance parameters to their best fit values and refitting the tagging SFs. The resulting uncertainty in the SFs is considered the statistical uncertainty. In cases where the SFs could not be determined, i.e., cases where the SFs are fixed to a value of 1 and the uncertainties are inflated to the range $[0.3, 3]$, the full uncertainty is treated as a statistical uncertainty. Statistical uncertainties of different jet flavors, tagging bins, and years are all treated as uncorrelated parameters when applied in the $t\bar{t}H(H \rightarrow c\bar{c})$ analysis.

The large majority of SFs for b, c, and light jets are within the range $[0.75, 1.5]$, with only few SFs outside this range. Uncertainties in the b jet SFs in the b jet enriched regions are generally small (of order 1–5%), and show continuous trends (i.e., SF values appear smooth for neighboring bins). Similarly, b jet SFs are well described in the c jet enriched bins C0–C4, but have somewhat larger uncertainties (of order 50%) in the L0 bin. SFs for c jets converge mostly well in c jet and light jet enriched bins. In higher b jet tagging bins (B1–B4), c jet SFs often cannot be constrained in the fit and are assigned a default value of one with large uncertainties. Similarly, light jet SFs cannot be well constrained in most c and b jet enriched bins, because of the low light-jet mistagging efficiencies.

B.3 Baseline event selection

The baseline event selection of this analysis is summarized in Table B.4. Corrections are applied to the simulated samples to account for differences in the jet energy scale and resolution, lepton selection efficiencies, and trigger efficiencies. Corrections for the variations in jet flavor identification efficiencies, discussed above, are also applied. Different selection criteria for different data-taking periods are motivated by changes in the trigger selection.

Table B.4: Baseline selection criteria in the 0L, 1L, and 2L channels. Where the selection criteria differ per year, they are quoted as 2016/2017/2018.

Selection criteria	0L channel	1L channel	2L channel
Number of leptons	0	1	2
Sign and flavor of leptons	—	$e^\pm, \mu^\pm$	$e^+e^-, \mu^\pm e^\mp, \mu^+\mu^-$
Min. p_T of p_T -leading electron [GeV]	—	29/30/30	25
Electron identification	—	Tight (80% efficiency)	Loose (90% efficiency)
Electron isolation	—	Tight (80% efficiency)	Loose (90% efficiency)
Min. p_T of p_T -leading muon [GeV]	—	26/29/26	25
Max. muon relative isolation	—	0.15	0.25
Min. $m_{ee/\mu\mu}$ [GeV]	—	—	20
Range of $m_{ee/\mu\mu}$ [GeV]	—	—	$<76, >106$
Min. p_T of jets [GeV]	25	25	25
Min. p_T of 6 th jet [GeV]	40	—	—
Max. $ \eta $ of jets	2.4	2.4	2.4
Min. number of jets	7	5	4
Min. number of b-tagged jets	1	1	1
Min. number of HF (b- or c-tagged) jets	3	3	3
Min. H_T [GeV]	500	—	—
Min. p_T^{miss} [GeV]	—	20	20

B.4 Neural network event classifier

The performance of the PART event classifier is summarized via the confusion matrices shown in Fig. B.2.

The fitted variable is the PART event classifier discriminant for the corresponding category as summarized in Table B.5. Several selections on the classifier discriminants define the analysis and validation regions (AR and VR), summarized in Fig. 5. In the 0L channel the classifier discriminant for the QCD multijet is used to remove the multijet background. The discriminant and the corresponding cut are shown in Fig. B.3. In all three channels, a cut on $\mathcal{D}_{t\bar{t}+\text{light}}$ is applied to reduce the overwhelming background from $t\bar{t}$ +light production, shown in Fig. B.4.

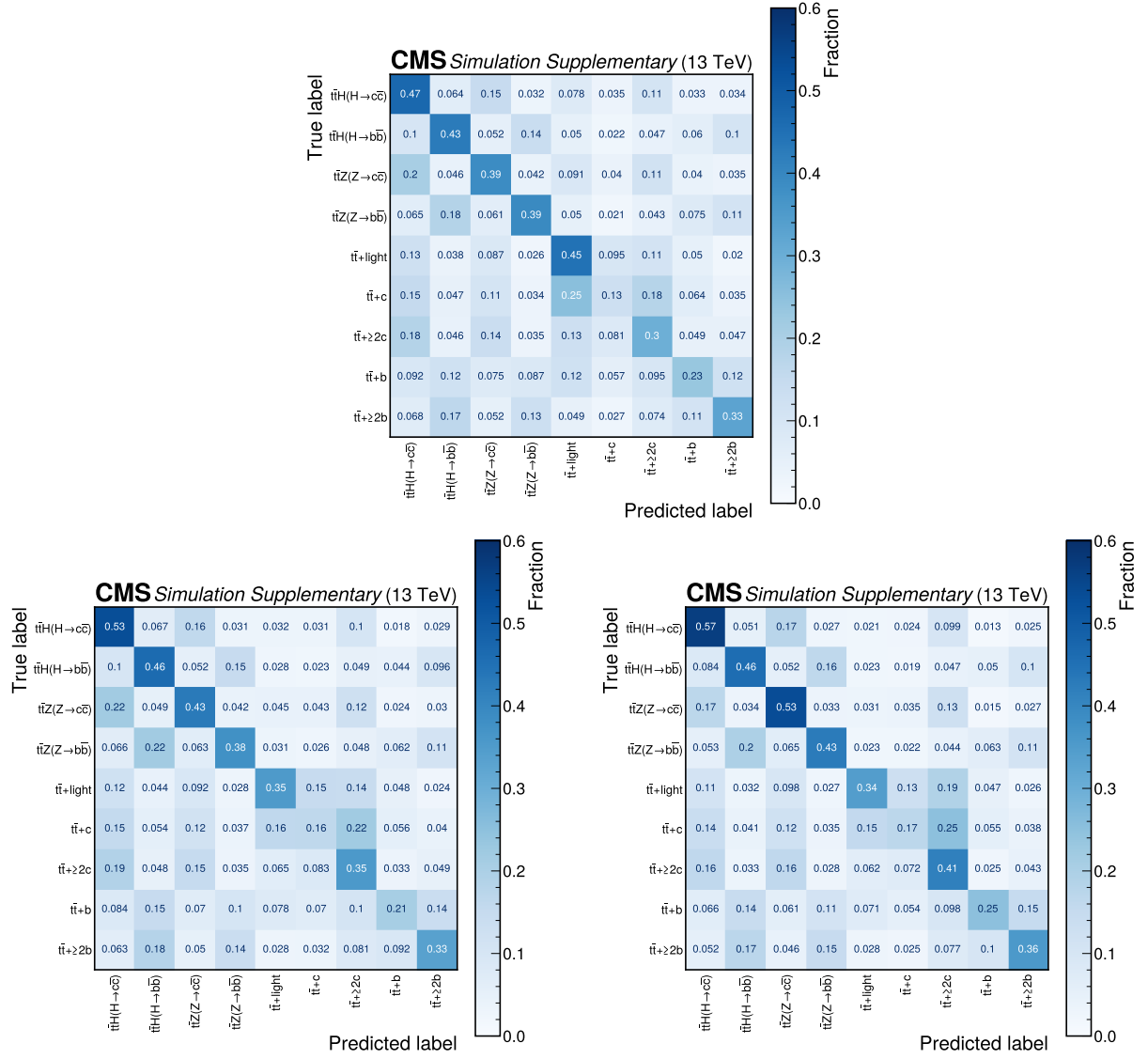


Figure B.2: Confusion matrices of the PART event classifier in the 0L (upper), 1L (lower left), and 2L (lower right) channels after the baseline selection. For each event, the predicted label is the process with the highest output discriminant. The event yield fractions are normalized per true label such that each row sums up to unity.

Table B.5: Definition of the PART event classifier discriminant for each category in the maximum likelihood fit.

Category	Discriminant
$H \rightarrow c\bar{c}$ SR	$\mathcal{D}_{t\bar{t}H(H \rightarrow c\bar{c})}$
$H \rightarrow b\bar{b}$ SR	$\mathcal{D}_{t\bar{t}H(H \rightarrow b\bar{b})}$
$Z \rightarrow c\bar{c}$ SR	$\mathcal{D}_{t\bar{t}Z(Z \rightarrow c\bar{c})}$
$Z \rightarrow b\bar{b}$ SR	$\mathcal{D}_{t\bar{t}Z(Z \rightarrow b\bar{b})}$
$t\bar{t} + \text{light}$ CR	$\mathcal{D}_{t\bar{t} + \text{light}} / \mathcal{D}_{t\bar{t} + \text{jets}}$
$t\bar{t} + c$ CR	$\mathcal{D}_{t\bar{t} + c} / \mathcal{D}_{t\bar{t} + \text{jets}}$
$t\bar{t} + \geq 2c$ CR	$\mathcal{D}_{t\bar{t} + \geq 2c} / \mathcal{D}_{t\bar{t} + \text{jets}}$
$t\bar{t} + b$ CR	$\mathcal{D}_{t\bar{t} + b} / \mathcal{D}_{t\bar{t} + \text{jets}}$
$t\bar{t} + \geq 2b$ CR	$\mathcal{D}_{t\bar{t} + \geq 2b} / \mathcal{D}_{t\bar{t} + \text{jets}}$

After these selections, the AR and VR, and the SRs and CRs are defined via requirements on $\mathcal{D}_{t\bar{t}X}$, summarized in Fig. B.5.

The event yields in the AR after the fit to data are summarized in Tables B.6–B.8 for the three individual channels, and in Tables B.9–B.10 for the full analysis.

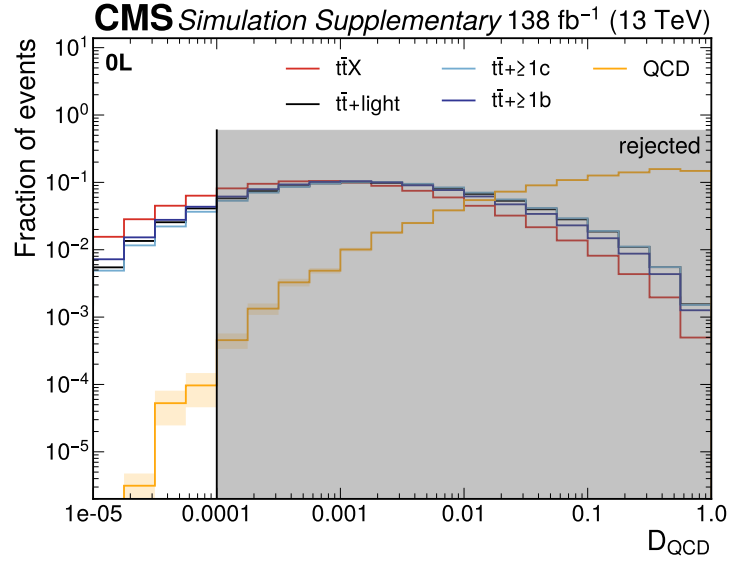


Figure B.3: Distribution of the PART $\mathcal{D}_{\text{QCD}}$ discriminant used in the 0L channel to remove the QCD background. The gray area indicates the region that is rejected in the analysis. The shaded band indicates the uncertainty in the QCD prediction due to limited size of simulated QCD multijet samples. All contributions are normalized to unity.

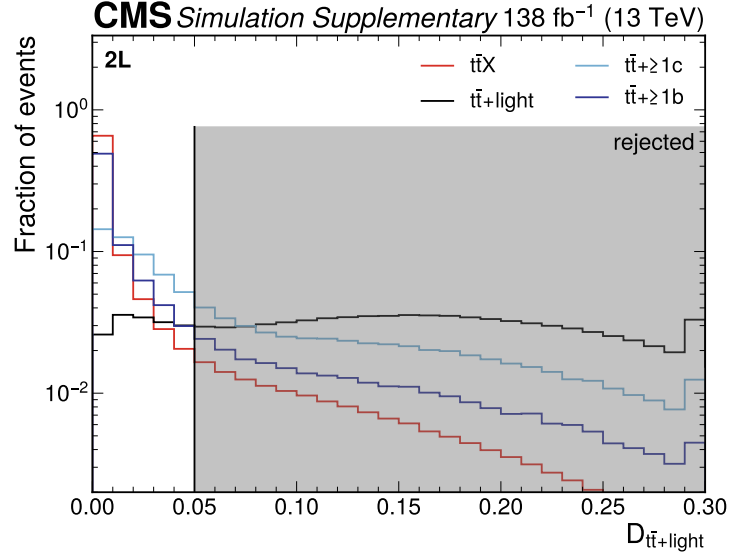


Figure B.4: Distribution of the PART $\mathcal{D}_{t\bar{t}+light}$ discriminant used to reduce the $t\bar{t}+light$ background in the 2L channel. The gray area indicates the region that is rejected in the analysis. All contributions are normalized to unity. The last bin includes the overflow.

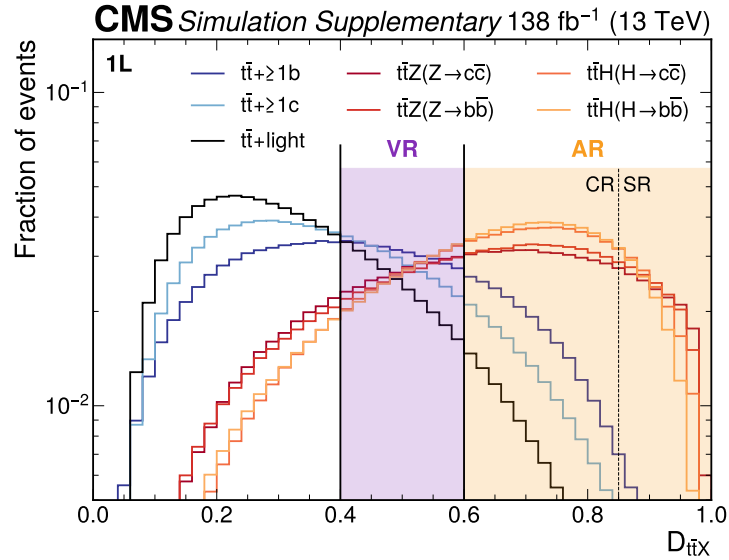


Figure B.5: Distribution of the PART $\mathcal{D}_{t\bar{t}X}$ discriminant used to define the different regions in the 1L channel. The purple (yellow) area indicates the region that is used for the validation (analysis). The dashed line indicates the separation of SRs and CRs in the analysis. All contributions are normalized to unity.

Table B.6: Event yields in the 2L channel. Values in brackets correspond to the pre-fit expectations.

Process	SR $t\bar{t}H(H \rightarrow c\bar{c})$	SR $t\bar{t}H(H \rightarrow b\bar{b})$	SR $t\bar{t}Z(Z \rightarrow c\bar{c})$	SR $t\bar{t}Z(Z \rightarrow b\bar{b})$	CR $t\bar{t} + \geq 2b$	CR $t\bar{t} + b$	CR $t\bar{t} + \geq 2c$	CR $t\bar{t} + c$	CR $t\bar{t} + \text{light}$
$t\bar{t}H(H \rightarrow c\bar{c})$	-2.5 ± 4.4 (1.5 $\pm$ 2.8)	-0.06 ± 0.62 (0.03 $\pm$ 0.37)	-0.5 ± 1.8 (0.3 $\pm$ 1.1)	-0.02 ± 0.35 (0.01 $\pm$ 0.21)	-0.13 ± 0.83 (0.08 $\pm$ 0.50)	-0.04 ± 0.51 (0.02 $\pm$ 0.31)	-1.2 ± 2.8 (0.7 $\pm$ 1.7)	-0.4 ± 1.5 (0.24 $\pm$ 0.97)	-4.4 ± 5.2 (2.7 $\pm$ 3.2)
$t\bar{t}H(H \rightarrow b\bar{b})$	2.4 ± 3.1 (2.7 $\pm$ 3.4)	20.2 ± 9.6 (22 $\pm$ 11)	1.3 ± 2.1 (1.4 $\pm$ 2.2)	6.4 ± 4.7 (7.1 $\pm$ 5.2)	37 ± 12 (40 $\pm$ 13)	18.6 ± 8.1 (20.8 $\pm$ 9.0)	4.1 ± 3.4 (4.4 $\pm$ 3.6)	1.8 ± 2.4 (2.1 $\pm$ 2.6)	45 ± 11 (50 $\pm$ 13)
$t\bar{t}Z(Z \rightarrow c\bar{c})$	1.9 ± 2.7	0.11 ± 0.64	9.9 ± 7.1	0.21 ± 0.90	0.4 ± 1.1	0.12 ± 0.71	4.3 ± 4.2	1.2 ± 2.2	14.2 ± 7.4
$t\bar{t}Z(Z \rightarrow b\bar{b})$	0.7 ± 2.1	3.8 ± 4.7	1.1 ± 2.7	16 ± 11	19 ± 11	9.1 ± 7.2	2.1 ± 3.1	0.9 ± 2.2	23 ± 10
$t\bar{t} + \geq 2b$	12.7 ± 7.9	45 ± 16	11.8 ± 7.4	52 ± 17	370 ± 42	121 ± 24	52 ± 15	14.3 ± 8.0	385 ± 40
$t\bar{t} + b$	19 ± 14	14 ± 13	16 ± 12	17 ± 14	120 ± 32	303 ± 56	54 ± 22	37 ± 19	727 ± 81
$t\bar{t} + \geq 2c$	67 ± 21	1.9 ± 3.7	63 ± 20	2.4 ± 3.3	16.0 ± 7.7	5.5 ± 5.6	214 ± 35	44 ± 15	524 ± 52
$t\bar{t} + c$	61 ± 28	1.7 ± 4.0	49 ± 24	3.4 ± 6.8	16 ± 11	23 ± 16	121 ± 37	166 ± 43	1290 ± 120
$t\bar{t} + \text{light}$	50 ± 14	1.7 ± 2.7	44 ± 12	1.8 ± 2.7	8.1 ± 4.7	11.2 ± 6.1	60 ± 14	54 ± 13	1470 ± 74
Other	15 ± 18	2.8 ± 7.3	24 ± 24	5.4 ± 9.7	22 ± 17	8.5 ± 8.1	32 ± 25	13 ± 14	313 ± 75
Total	228 ± 14	90.7 ± 7.9	220 ± 14	103.6 ± 9.1	608 ± 22	499 ± 19	541 ± 27	332 ± 18	4790 ± 110
Data	236	93	204	92	605	463	546	343	4784

Table B.7: Event yields in the 1L channel. Values in brackets correspond to the pre-fit expectations.

Process	SR $t\bar{t}H(H \rightarrow c\bar{c})$	SR $t\bar{t}H(H \rightarrow b\bar{b})$	SR $t\bar{t}Z(Z \rightarrow c\bar{c})$	SR $t\bar{t}Z(Z \rightarrow b\bar{b})$	CR $t\bar{t} + \geq 2b$	CR $t\bar{t} + b$	CR $t\bar{t} + \geq 2c$	CR $t\bar{t} + c$	CR $t\bar{t} + \text{light}$
$t\bar{t}H(H \rightarrow c\bar{c})$	-16 ± 22 (10 $\pm$ 14)	-0.5 ± 3.6 (0.3 $\pm$ 2.1)	-3.1 ± 8.9 (1.9 $\pm$ 5.4)	-0.2 ± 1.9 (0.1 $\pm$ 1.1)	-1.2 ± 2.6 (0.7 $\pm$ 1.5)	-0.5 ± 1.8 (0.3 $\pm$ 1.0)	-11.7 ± 8.8 (7.0 $\pm$ 5.3)	-5.4 ± 5.9 (3.3 $\pm$ 3.6)	-24 ± 13 (14.8 $\pm$ 7.7)
$t\bar{t}H(H \rightarrow b\bar{b})$	21 ± 18 (23 $\pm$ 19)	166 ± 55 (181 $\pm$ 60)	9 ± 11 (10 $\pm$ 12)	43 ± 25 (47 $\pm$ 27)	264 ± 31 (284 $\pm$ 34)	139 ± 22 (153 $\pm$ 25)	52 ± 12 (55 $\pm$ 13)	35 ± 10 (38 $\pm$ 11)	327 ± 32 (356 $\pm$ 35)
$t\bar{t}Z(Z \rightarrow c\bar{c})$	16 ± 16	1.1 ± 4.1	59 ± 35	1.5 ± 4.9	3.5 ± 3.6	1.6 ± 2.5	37 ± 12	18.1 ± 8.6	78 ± 18
$t\bar{t}Z(Z \rightarrow b\bar{b})$	6 ± 12	32 ± 28	8 ± 14	114 ± 58	136 ± 28	70 ± 20	25 ± 11	19.2 ± 9.7	166 ± 29
$t\bar{t} + \geq 2b$	109 ± 48	387 ± 91	85 ± 41	360 ± 88	2760 ± 120	957 ± 67	633 ± 51	293 ± 34	2830 ± 110
$t\bar{t} + b$	198 ± 96	205 ± 97	168 ± 88	165 ± 87	1300 ± 110	2700 ± 170	841 ± 88	719 ± 81	5760 ± 240
$t\bar{t} + \geq 2c$	470 ± 110	26 ± 24	389 ± 99	19 ± 21	153 ± 26	60 ± 18	2080 ± 110	718 ± 63	3400 ± 140
$t\bar{t} + c$	700 ± 190	61 ± 54	470 ± 150	45 ± 46	256 ± 48	291 ± 59	1910 ± 150	2680 ± 180	9220 ± 330
$t\bar{t} + \text{light}$	780 ± 110	73 ± 33	605 ± 94	69 ± 33	205 ± 24	226 ± 29	1180 ± 65	1326 ± 70	12620 ± 220
Other	190 ± 120	43 ± 48	320 ± 160	58 ± 55	249 ± 50	136 ± 33	550 ± 86	423 ± 70	3080 ± 190
Total	2470 ± 92	993 ± 52	2115 ± 80	875 ± 48	5330 ± 110	4580 ± 110	7300 ± 200	6230 ± 190	37450 ± 530
Data	2411	983	2108	879	5372	4594	7317	6209	37497

Table B.8: Event yields in the 0L channel. Values in brackets correspond to the pre-fit expectations.

Process	SR $t\bar{t}H(H \rightarrow c\bar{c})$	SR $t\bar{t}H(H \rightarrow b\bar{b})$	SR $t\bar{t}Z(Z \rightarrow c\bar{c})$	SR $t\bar{t}Z(Z \rightarrow b\bar{b})$	CR $t\bar{t} + \geq 2b$	CR $t\bar{t} + b$	CR $t\bar{t} + \geq 2c$	CR $t\bar{t} + c$	CR $t\bar{t} + \text{light}$
$t\bar{t}H(H \rightarrow c\bar{c})$	-9 ± 13 (5.5 $\pm$ 8.1)	-0.4 ± 2.5 (0.2 $\pm$ 1.4)	-1.6 ± 5.0 (1.0 $\pm$ 3.0)	-0.1 ± 1.4 (0.08 $\pm$ 0.79)	-0.7 ± 1.9 (0.4 $\pm$ 1.1)	-0.3 ± 1.4 (0.17 $\pm$ 0.79)	-3.4 ± 4.7 (2.0 $\pm$ 2.8)	-0.5 ± 1.9 (0.3 $\pm$ 1.1)	-17 ± 10 (10.2 $\pm$ 6.2)
$t\bar{t}H(H \rightarrow b\bar{b})$	12 ± 10 (13 $\pm$ 11)	128 ± 38 (137 $\pm$ 41)	5.4 ± 6.5 (5.9 $\pm$ 7.1)	31 ± 16 (34 $\pm$ 17)	140 ± 23 (151 $\pm$ 24)	62 ± 15 (68 $\pm$ 16)	14.9 ± 6.5 (15.8 $\pm$ 6.9)	2.9 ± 2.8 (3.1 $\pm$ 3.0)	185 ± 23 (201 $\pm$ 25)
$t\bar{t}Z(Z \rightarrow c\bar{c})$	8.0 ± 9.0	0.8 ± 2.9	36 ± 21	1.3 ± 3.6	1.9 ± 2.6	1.0 ± 2.0	10.4 ± 6.7	2.0 ± 2.9	51 ± 14
$t\bar{t}Z(Z \rightarrow b\bar{b})$	3.1 ± 6.5	22 ± 18	4.7 ± 8.3	87 ± 40	62 ± 19	28 ± 13	6.2 ± 5.4	1.5 ± 2.7	75 ± 19
$t\bar{t} + \geq 2b$	73 ± 32	336 ± 73	55 ± 28	320 ± 70	1548 ± 97	452 ± 50	178 ± 30	28 ± 11	1677 ± 89
$t\bar{t} + b$	86 ± 47	96 ± 49	70 ± 43	88 ± 50	405 ± 60	742 ± 86	159 ± 37	45 ± 20	2040 ± 130
$t\bar{t} + \geq 2c$	296 ± 81	22 ± 21	260 ± 75	20 ± 19	74 ± 22	30 ± 15	653 ± 72	85 ± 25	2410 ± 130
$t\bar{t} + c$	163 ± 59	21 ± 20	113 ± 48	16 ± 17	49 ± 18	44 ± 19	180 ± 39	113 ± 30	2520 ± 140
$t\bar{t} + \text{light}$	213 ± 42	27 ± 15	165 ± 36	21 ± 13	44 ± 11	43 ± 12	122 ± 20	50 ± 13	4310 ± 120
Other	39 ± 40	13 ± 20	106 ± 67	18 ± 23	32 ± 19	24 ± 15	52 ± 29	17 ± 16	565 ± 88
Total	883 ± 50	665 ± 42	814 ± 47	602 ± 40	2357 ± 74	1426 ± 63	1372 ± 64	343 ± 26	13800 ± 310
Data	898	668	831	622	2345	1435	1382	357	13733

Table B.9: Event yields in the full analysis, separated in the SRs and CRs. Values in brackets correspond to the pre-fit expectations.

Process	SR $t\bar{t}H(H \rightarrow c\bar{c})$	SR $t\bar{t}H(H \rightarrow b\bar{b})$	SR $t\bar{t}Z(Z \rightarrow c\bar{c})$	SR $t\bar{t}Z(Z \rightarrow b\bar{b})$	CR $t\bar{t} + \geq 2b$	CR $t\bar{t} + b$	CR $t\bar{t} + \geq 2c$	CR $t\bar{t} + c$	CR $t\bar{t} + \text{light}$
$t\bar{t}H(H \rightarrow c\bar{c})$	-27 ± 40 (17 $\pm$ 25)	-0.9 ± 6.7 (0.5 $\pm$ 3.8)	-5 ± 16 (3.2 $\pm$ 9.5)	-0.3 ± 3.7 (0.2 $\pm$ 2.1)	-2.0 ± 5.4 (1.2 $\pm$ 3.1)	-0.8 ± 3.6 (0.5 $\pm$ 2.1)	-16 ± 16 (9.8 $\pm$ 9.8)	-6.3 ± 9.3 (3.9 $\pm$ 5.7)	-46 ± 28 (28 $\pm$ 17)
$t\bar{t}H(H \rightarrow b\bar{b})$	35 ± 31 (38 $\pm$ 34)	310 ± 100 (340 $\pm$ 110)	16 ± 20 (17 $\pm$ 21)	81 ± 45 (88 $\pm$ 49)	441 ± 65 (475 $\pm$ 71)	220 ± 45 (242 $\pm$ 50)	71 ± 22 (75 $\pm$ 24)	40 ± 15 (43 $\pm$ 17)	557 ± 67 (607 $\pm$ 73)
$t\bar{t}Z(Z \rightarrow c\bar{c})$	25 ± 28	2.0 ± 7.6	105 ± 63	2.9 ± 9.4	5.8 ± 7.3	2.7 ± 5.3	51 ± 23	21 ± 14	143 ± 40
$t\bar{t}Z(Z \rightarrow b\bar{b})$	10 ± 21	57 ± 51	14 ± 25	220 ± 110	218 ± 58	108 ± 40	34 ± 20	22 ± 15	263 ± 58
$t\bar{t} + \geq 2b$	194 ± 88	770 ± 180	152 ± 76	730 ± 170	4680 ± 260	1530 ± 140	862 ± 95	335 ± 53	4890 ± 240
$t\bar{t} + b$	300 ± 160	320 ± 160	250 ± 140	270 ± 150	1830 ± 200	3740 ± 310	1050 ± 150	800 ± 120	8520 ± 450
$t\bar{t} + \geq 2c$	830 ± 210	50 ± 49	710 ± 190	41 ± 43	244 ± 56	96 ± 39	2950 ± 220	850 ± 100	6330 ± 320
$t\bar{t} + c$	920 ± 270	84 ± 78	640 ± 230	64 ± 70	321 ± 77	358 ± 94	2210 ± 230	2960 ± 250	13030 ± 590
$t\bar{t} + \text{light}$	1050 ± 160	102 ± 51	810 ± 140	92 ± 49	257 ± 39	280 ± 47	1362 ± 99	1430 ± 96	18390 ± 410
Other	240 ± 180	58 ± 76	450 ± 250	82 ± 88	303 ± 87	169 ± 56	630 ± 140	453 ± 100	3950 ± 350
Total	3580 ± 160	1750 ± 100	3150 ± 140	1580 ± 97	8300 ± 210	6500 ± 200	9210 ± 290	6910 ± 240	56040 ± 950
Data	3545	1744	3143	1593	8322	6492	9245	6909	56014

Table B.10: Event yields in the full analysis, separated per lepton channel. Values in brackets correspond to the pre-fit expectations.

Process	2L	1L	0L	Total
$t\bar{t}H(H \rightarrow c\bar{c})$	-9 ± 18 (6 $\pm$ 11)	-62 ± 69 (38 $\pm$ 42)	-33 ± 42 (20 $\pm$ 25)	-100 ± 130 (64 $\pm$ 78)
$t\bar{t}H(H \rightarrow b\bar{b})$	137 ± 56 (151 $\pm$ 62)	1060 ± 220 (1150 $\pm$ 240)	580 ± 140 (630 $\pm$ 150)	1770 ± 410 (1930 $\pm$ 450)
$t\bar{t}Z(Z \rightarrow c\bar{c})$	32 ± 27	210 ± 110	112 ± 65	360 ± 200
$t\bar{t}Z(Z \rightarrow b\bar{b})$	75 ± 53	580 ± 210	290 ± 130	940 ± 400
$t\bar{t} + \geq 2b$	1060 ± 180	8420 ± 650	4670 ± 480	14100 ± 1300
$t\bar{t} + b$	1310 ± 260	12100 ± 1000	3730 ± 530	17100 ± 1800
$t\bar{t} + \geq 2c$	940 ± 160	7320 ± 610	3850 ± 460	12100 ± 1200
$t\bar{t} + c$	1730 ± 290	15600 ± 1200	3220 ± 390	20600 ± 1900
$t\bar{t} + \text{light}$	1700 ± 140	17080 ± 670	4990 ± 280	23800 ± 1100
Other	430 ± 200	5040 ± 810	870 ± 320	6300 ± 1300
Total	7410 ± 240	67300 ± 1400	22270 ± 720	97000 ± 2400
Data	7366	67370	22271	97007

B.5 Systematic uncertainties

Systematic uncertainties are evaluated by appropriate variations of the signal and background simulations. The uncertainty sources affect either the rate or the discriminant shape of the signal or background processes, or both. They are taken into account via nuisance parameters in the final profile likelihood fit. The effects from the same source are treated as fully correlated among the different categories.

The considered sources of uncertainties are listed in Table B.11 and described in detail in the following sections, grouped by experimental uncertainties in Section B.6 and modeling uncertainties in Section B.7. Their impact on the final result is discussed in Section B.9.

As for the final statistical inference, the templates corresponding to individual years are merged to obtain only one template. We then consider the appropriate correlation scheme in the following way. For correlated systematic uncertainties the templates are varied simultaneously in all years, while for decorrelated systematics the template of the corresponding year(s) are varied, and for all other years the nominal template is considered. This way, partial effects are correctly taken into account as partial variations.

Table B.11: Summary of the systematic uncertainty sources in the measurement. The first column lists the source of the uncertainty. The second (third) column indicates the treatment of correlations of the uncertainties between different data-taking periods (processes), where $\checkmark$ means fully correlated, $\sim$ means partially correlated (i.e., contains sub-sources that are either fully correlated or uncorrelated), and $\times$ means uncorrelated. The last column indicates whether the uncertainties are applied to all processes or only a subset.

	Source	Corr. (period)	Corr. (process)	Processes
Experimental	Integrated luminosity	$\sim$	$\checkmark$	all
	Electron reconstruction and identification	$\checkmark$	$\checkmark$	all
	Muon reconstruction and identification	$\checkmark$	$\checkmark$	all
	Trigger efficiencies	$\times$	$\checkmark$	all
	Pileup reweighting	$\checkmark$	$\checkmark$	all
	Jet energy scale (11 sources)	$\sim$	$\checkmark$	all
	Jet energy resolution	$\times$	$\checkmark$	all
	Unclassified p_T^{miss}	$\times$	$\checkmark$	all
	Jet flavor tagging	$\sim$	$\checkmark$	all
Modeling	Incl. cross sections & normalization	$\checkmark$	$\sim$	all
	μ_R scale	$\checkmark$	$\times$	$t\bar{t} + \text{jets}$, $t\bar{t}X$, single t
	μ_F scale	$\checkmark$	$\times$	$t\bar{t} + \text{jets}$, $t\bar{t}X$, single t
	PDF shape	$\checkmark$	$\times$	$t\bar{t} + \text{jets}$, $t\bar{t}X$
	PS scales: ISR	$\checkmark$	$\times$	$t\bar{t} + \text{jets}$, $t\bar{t}X$, single t
	PS scales: FSR	$\checkmark$	$\times$	$t\bar{t} + \text{jets}$, $t\bar{t}X$, single t
	ME-PS matching (h_{damp})	$\checkmark$	$\times$	$t\bar{t} + \text{jets}$
	ME (4 vs. 5 flavor scheme)	$\checkmark$	$\times$	$t\bar{t} + \geq 1b$

B.6 Experimental uncertainties

- **Luminosity:** The integrated luminosities of the data-taking periods are individually measured with uncertainties of 1.2, 2.3, and 2.5% for 2016, 2017, and 2018 data-taking periods, respectively [30–32]. The uncertainty in the integrated luminosity of the combined data set is 1.6%, when taking into account the correlations between the periods.

- **Lepton scale factors:** Separate p_T and η dependent uncertainties are assigned to the reconstruction and identification efficiencies for electrons in the simulation. Similarly, the muon tracking, identification, and isolation efficiencies are estimated. The associated uncertainties are propagated to the final discriminant distributions as a total shape uncertainty estimated from the sum of all sources and of the statistical and systematic components, separately for electrons and muons. The impact of the lepton calibration uncertainties in the final result is negligible.
- **Trigger scale factors:** The trigger efficiency scale factors are varied within their uncertainties, separately for each lepton number and flavor combination and the hadronic trigger selection.
- **Pileup reweighting:** The prediction of number of pileup interactions in simulation is performed with a total inelastic pp cross section of 69.2 mb. Changes in the assumed pileup multiplicity are estimated by varying the total inelastic cross section by $\pm 4.6\%$ [92]. This uncertainty is treated as fully correlated between data-taking periods.
- **L1 prefiring issue:** During the 2016–2017 data-taking periods, a gradual shift in the timing of the inputs of the ECAL L1 trigger in the forward endcap region ($|\eta| > 2.4$) led to a specific inefficiency, known as “prefiring”. A similar effect is present for the muon system because of its limited time resolution, which was most pronounced in 2016 but also impacted data collected in 2017–2018. Corrections for this effect are applied to simulated events, and 20% of the corrections are assigned as the associated uncertainties.
- **Jet energy scale:** Uncertainties in the determination of the jet energy scale are taken into account by shifting the jet energy scale applied to the reconstructed jets in the simulation up and down by one standard deviation, separately for each of several sources of uncertainty, such as the overall energy scale, differences in flavor response, and residual differences between energy scale measurements [46]. Some of these sources are treated separately per data-taking period, while some are correlated for all periods.
- **Jet energy resolution:** Uncertainties in the jet energy resolution are evaluated by increasing or decreasing the difference between jet energies at reconstructed and particle level, or by smearing the measured jet energy in case no matching particle-level jet could be found [46]. This uncertainty is uncorrelated between data-taking periods.
- **Unclassified p_T^{miss} :** An additional uncertainty in p_T^{miss} is derived by varying the energies of reconstructed particles not clustered into jets.
- **Jet flavor tagging:** Uncertainties in the flavor tagging calibration described in Section B.2 are taken into account. The flavor tagging uncertainties include statistical uncertainties in the derived SFs, effects due to the choice of the μ_F and μ_R scales, variations in PS ISR and FSR in PYTHIA, uncertainties in the fraction of b and c jets in the simulated W+jets and Z+jets events, jet energy scale and resolution uncertainties, and pileup uncertainties. The statistical uncertainties in the scale factors are treated as uncorrelated, while all the other uncertainties in the scale factors are treated as fully correlated.

B.7 Modeling uncertainties

This measurement is strongly affected by uncertainties in the modeling of the $t\bar{t}$ +jets background processes, especially the $t\bar{t}+\geq 1b$ processes. Variations applied to the $t\bar{t}$ +jets background processes are defined such that the predicted yields in the inclusive phase space region before acceptance effects or any event selection remain constant for the individual processes. This procedure ensures that the modeling uncertainties for the $t\bar{t}$ +jets processes only have an effect on the selection efficiency, and not on the cross section of the processes. The normalization of the individual processes are degrees of freedom in the binned profile likelihood fit. Furthermore, the uncertainty in the overall normalization of the $t\bar{t}$ process is covered with separate systematic uncertainties, as detailed below.

All modeling uncertainties are correlated between the data-taking years. Some uncertainties are correlated between processes.

- **Inclusive cross sections:** The expectation for the inclusive signal and background cross sections are derived from theoretical predictions of at least NLO accuracy. Uncertainties affecting these normalizations are split into a component due to the μ_R and μ_F scale uncertainties in the ME calculation and a component due to the PDF set and choice of the strong coupling constant α_S (PDF+ α_S) for the $t\bar{t}H$ signal and the $t\bar{t}Z$ process. These uncertainties are taken into account as rate-changing uncertainties in the final fit and are on the order of 9% for $t\bar{t}Z$ [93] and are split into three components for $t\bar{t}H$ production [89], taking into account the effects from variations of the scales ($+5.8\% - 9.2\%$), α_S (2%), and the PDFs (3%).
- **Branching fractions:** For the $t\bar{t}H$ process, several rate-changing uncertainties are assigned to the signal and background contributions, depending on the final state. The uncertainties are taken from Ref. [89] and denote about 1.3% (10%) in total for $H \rightarrow b\bar{b}$ ($H \rightarrow c\bar{c}$) decays.
- **Renormalization and factorization scales:** Uncertainties due to the renormalization scale μ_R and the factorization scale μ_F in the ME generators are modeled by shifting the scales independently up and down by a factor of two. These uncertainties are treated separately for each process and for each of the seven $t\bar{t}$ +jets background components.
- **PDF shape:** The NNPDF3.1 NNLO PDF set is used for the description of the substructure of the colliding protons in simulation. The shape variations of the fit distribution are evaluated by reweighting the simulated events with the replicas of the PDF set. We calculate the root-mean-square of all residuals for the 4FS PDF set, used for the $t\bar{t}+\geq 1b$ backgrounds. For the other processes, using the 5FS PDF set, the variations correspond to the eigenvectors of the PDF fit covariance matrix, and individual uncertainties are obtained from each eigenvector. Each eigenvector variation is treated as one separate uncertainty in the fit. An additional uncertainty from the value of α_S , used in the PDFs, is included. These uncertainties are treated as correlated for all processes of common PDF flavor schemes.
- **PS scales ISR/FSR:** In order to estimate the impact of the choice of scale at which α_S is evaluated in the PS simulation, the scales in the shower simulation are varied up and down by a factor of two, independently for ISR and FSR. For both ISR and FSR, the uncertainties are split into 8 separate components. We individually vary the scales and nonsingular terms for the splitting kernels $g \rightarrow gg$, $g \rightarrow q\bar{q}$, $q \rightarrow qg$, $x \rightarrow xg$, where $x = t, b$, as implemented in PYTHIA v8 [94]. These uncertainties are considered as uncorrelated for all processes.

- **ME-PS matching (h_{damp}):** In the POWHEG generator, the scale that separates the phase space of the first QCD emission into soft and hard parts is controlled via the h_{damp} parameter. For the CP5 tune, when POWHEG is matched to the PYTHIA v8 [94] PS, the central value of h_{damp} is set to $h_{\text{damp}} = 1.379m_t$, and the uncertainties are estimated with varied values of $h_{\text{damp}} = 2.305m_t$ and $0.874m_t$ for the $t\bar{t}$ and $t\bar{t} + \geq 1b$ simulations. The alternative predictions with varied h_{damp} values are obtained via an ML-reweighting approach [95]. This uncertainty is treated as uncorrelated between the different $t\bar{t} + \text{jets}$ processes.
- **Background normalization:** To account for the known issues in the modeling of different background processes, we assign the following normalization uncertainties: 25% for single top quark, 100% for tWZ due to the discrepancies between prediction and measurements [96], 6.8% for $t\bar{t}W$ [97], and 50% for the relative $t\bar{t} + j_{bb}$ and $t\bar{t} + j_{cc}$ contributions with respect to $t\bar{t} + j_b$ and $t\bar{t} + j_c$, respectively, to account for the limited knowledge of the rate of collinear gluon splitting.
- **$t\bar{t}b\bar{b}$ DPS normalization:** The $t\bar{t}b\bar{b}$ DPS cross section is not precisely known and an estimate of the effective cross section for DPS is used, which is process dependent. Different measurements of this effective cross section range between 10–30 mb [90], while the PYTHIA reference value is 30 mb. Given the limited knowledge of the effective cross section value for $t\bar{t}b\bar{b}$ DPS, a 50% normalization uncertainty is applied to the $t\bar{t}b\bar{b}$ DPS contributions.
- **$t\bar{t} + \geq 1b$ modeling differences:** The nominal model for the estimation of the $t\bar{t} + \geq 1b$ background relies on the NLO ME description of $t\bar{t} + \geq 2b$ using POWHEG-BOX-RES, interfaced with PYTHIA for parton showering and hadronization. Dedicated measurements of $t\bar{t} + \geq 1b$ production show that this simulation approach is able to describe the most relevant observables in data [56], when taking into account the systematic modeling uncertainties described previously. Nevertheless, in order to provide additional freedom for the background model, the difference between the nominal model and the description of $t\bar{t} + \geq 1b$ with the $t\bar{t}$ -inclusive NLO POWHEG model, interfaced with PYTHIA, is used as a systematic uncertainty. The variations are normalized to the nominal event yield after baseline selection. This alternative $t\bar{t} + \geq 1b$ model does not describe relevant physics objects significantly differently than the nominal background model. This uncertainty is considered decorrelated for the $t\bar{t} + j_b$ processes and decorrelated among all four SRs.

B.8 Validation of the background model

A signal-depleted sideband validation region (VR), with a partition into a control-like region for $0.40 < \mathcal{D}_{t\bar{t}X} < 0.58$ and a signal-like region for $0.58 < \mathcal{D}_{t\bar{t}X} < 0.60$, analogous to the AR partition into a CR and a SR, is used to validate the background estimation strategy, and good agreement is observed between data and estimated backgrounds, as shown in Fig. B.6. Each region in the VR is defined such that the purity of the background components is as close as possible to those in the CRs and SRs.

B.9 Additional results

The production rates of the signal processes and the normalization factors of the $t\bar{t}$ background components are determined via a binned profile likelihood fit to data in all the SRs and CRs. The fitted observables are described in Section B.4. Figure B.7 shows the observed yields in each bin of the event classifier discriminant for all CRs and SRs, along with the fitted signal and background yields. Figures B.8–B.9 summarize the results of the measurements of the

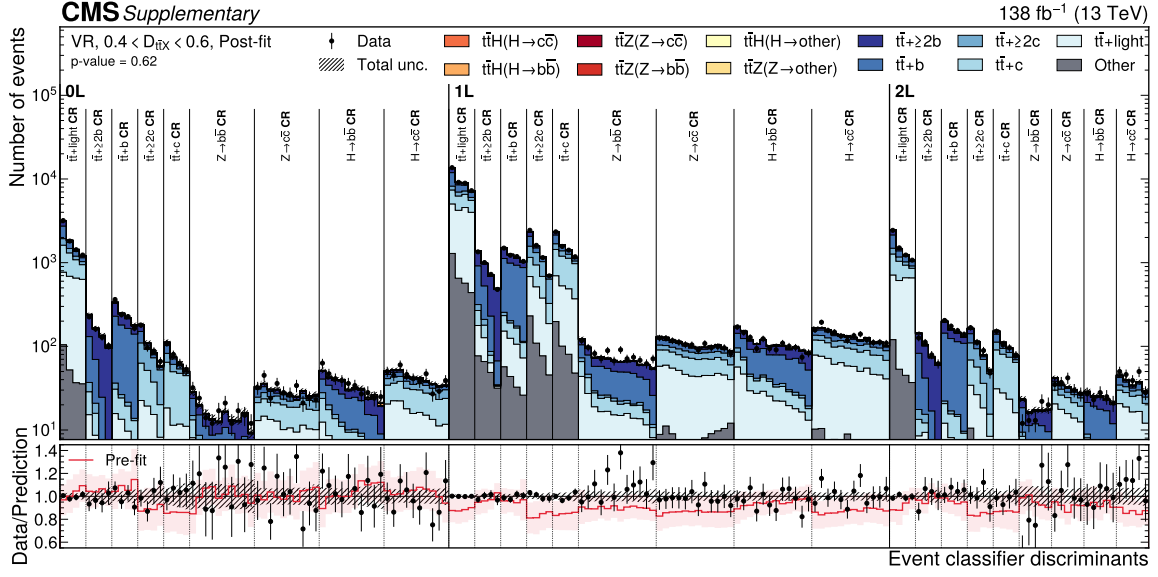


Figure B.6: Distributions of the PART discriminants in data (points) and predicted signal and backgrounds (colored histograms) after the maximum likelihood fit to data in the VR, defined by $0.4 < D_{\text{ttX}} < 0.6$. The vertical bars on the points represent the statistical uncertainties in data. The hatched band represents the total uncertainty in the sum of the signal and background predictions. The lower panel shows the ratio of the data to the sum of the signal and background predictions. The ratio of the pre-fit expectation to the sum of the signal and background predictions after the fit is shown as a red line in the lower panel, including the pre-fit uncertainties as a shaded band.

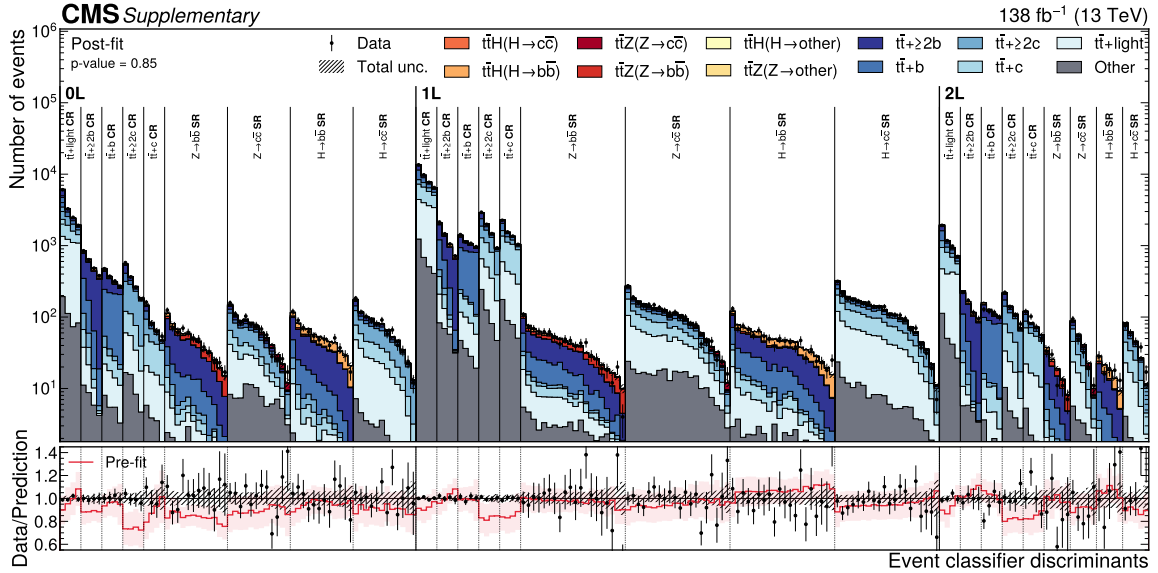


Figure B.7: Distributions of the PART discriminants in data (points) and predicted signal and backgrounds (colored histograms) after the maximum likelihood fit to data. The vertical bars on the points represent the statistical uncertainties in data. The hatched band represents the total uncertainty in the sum of the signal and background predictions. The lower panel shows the ratio of the data to the sum of the signal and background predictions. The ratio of the pre-fit expectation to the sum of the signal and background predictions after the fit is shown as a red line in the lower panel, including the pre-fit uncertainties as a shaded band.

$t\bar{t}Z(Z \rightarrow c\bar{c})$ and $t\bar{t}Z(Z \rightarrow b\bar{b})$ signal strengths, respectively, obtained from the simultaneous fit of all four signal strength parameters and all SRs and CRs. Figure B.10 shows the contributions from the individual channels for the best fit values of $\mu_{t\bar{t}H(H \rightarrow b\bar{b})}$.

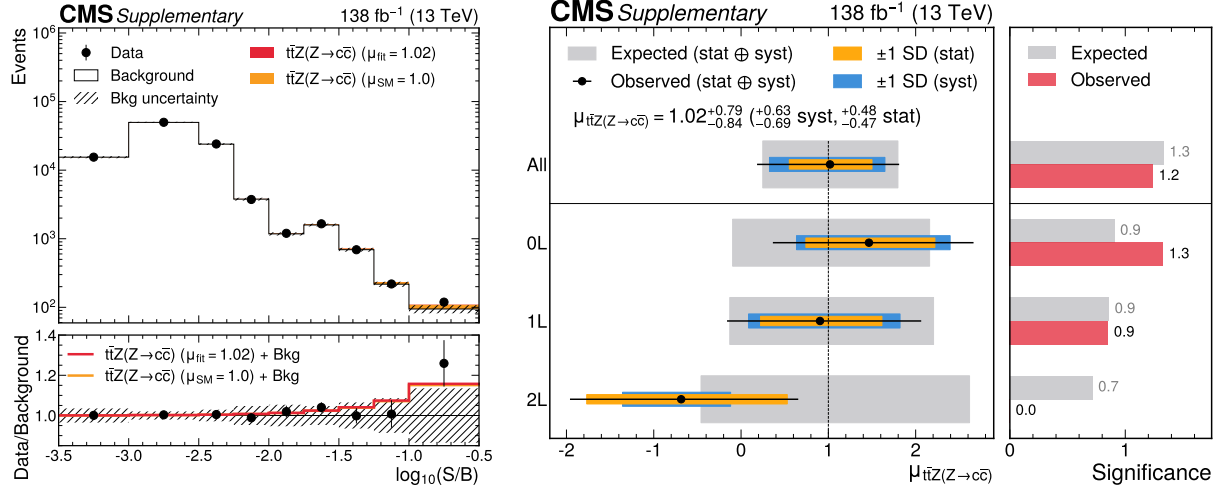


Figure B.8: On the left, observed and expected event yields from all SRs and CRs as a function of $\log_{10}(S/B)$, where S are the observed $t\bar{t}Z(Z \rightarrow c\bar{c})$ yields, and B are the total background yields in the combined fit to data. The signals are shown for the best fit signal strength (red), and the SM prediction, $\mu = 1$ (orange). The lower panel shows the ratio of the data to the post-fit background prediction, compared to the signal-plus-background predictions. On the right, fit results of $\mu_{t\bar{t}Z(Z \rightarrow c\bar{c})}$ in the combination of channels (first row) and the channels individually (lower rows). The left panel shows the observed signal strength, compared to the expected results. The right panel shows the expected and observed significance.

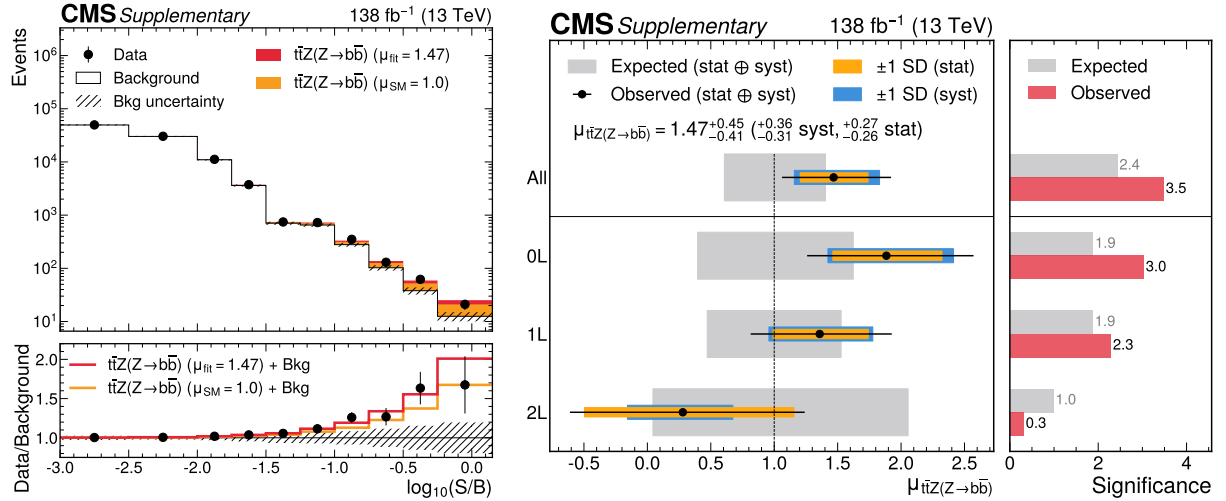


Figure B.9: On the left, observed and expected event yields from all SRs and CRs as a function of $\log_{10}(S/B)$, where S are the observed $t\bar{t}Z(Z \rightarrow b\bar{b})$ yields, and B are the total background yields in the combined fit to data. The signals are shown for the best fit signal strength (red), and the SM prediction, $\mu = 1$ (orange). The lower panel shows the ratio of the data to the post-fit background prediction, compared to the signal-plus-background predictions. On the right, fit results of $\mu_{t\bar{t}Z(Z \rightarrow b\bar{b})}$ in the combination of channels (first row) and the channels individually (lower rows). The left panel shows the observed signal strength, compared to the expected results. The right panel shows the expected and observed significance.

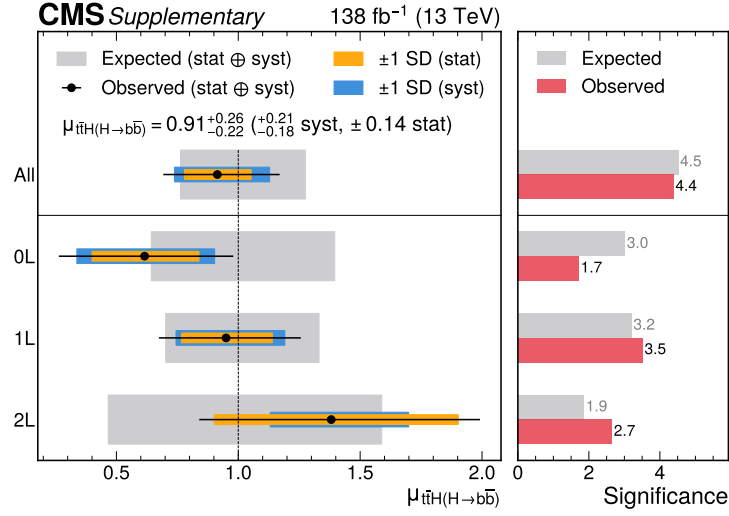


Figure B.10: Fit results of $\mu_{\text{ttH}(H \rightarrow b\bar{b})}$. The left panel shows the observed signal strength, compared to the expected results. The right panel shows the expected and observed significance.

The result is interpreted in the κ -framework [88, 89]. The one-dimensional likelihood scan for κ_c is shown in Fig. B.11, both for a fixed and a floating κ_b value.

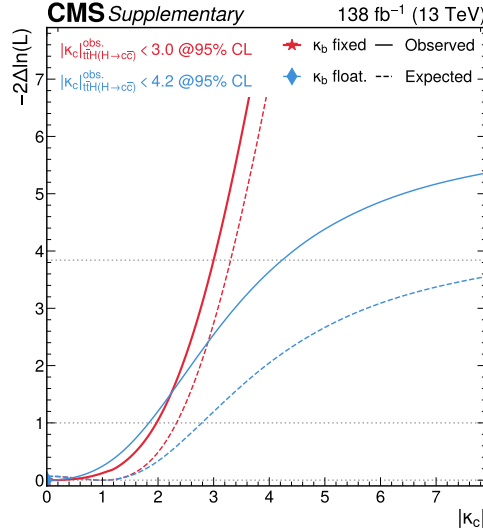


Figure B.11: Likelihood scans of κ_c with fixed $\kappa_b = 1$ (red) and floating κ_b (blue). The 68% and 95% CL intervals are indicated by the horizontal dotted lines.

The search is combined with a previous search in the VH channel [27]. All uncertainties in experimental effects, such as jet energy scale and resolution, lepton identification efficiencies, the modeling of detector effects, pileup and p_T^{miss} modeling, and the integrated luminosity are correlated. The flavor (mis-)tagging scale factors of the merged and resolved VH analyses are treated as uncorrelated with this measurement because of the differences in jet tagging algorithms and jet cone sizes, as well as in calibration methods. All uncertainties in the background and signal modeling are considered uncorrelated as well, since the main background in the VH analysis, Z+jets and W+jets production in association with heavy-flavor jets, and the VH signal contribution are negligible for this analysis. The dominant systematic uncertainties in each measurement are the normalization and modeling of the background components, which are negligible in the respective other measurement. Theoretical uncertainties such as in the Higgs boson branching fraction and production cross section are correlated. Each input mea-

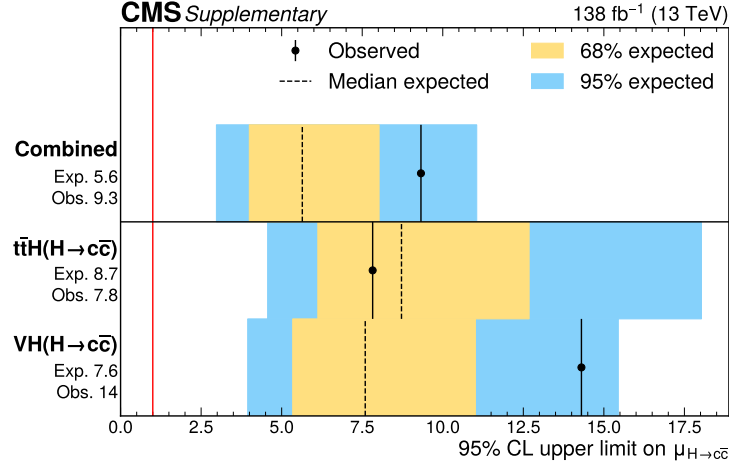


Figure B.12: The 95% CL upper limits on $\mu_{H \rightarrow c\bar{c}}$. The blue and yellow bands indicate the expected 68% and 95% CL regions, respectively, under the background-only hypothesis. The vertical red line indicates the SM value $\mu_{H \rightarrow c\bar{c}} = 1$.

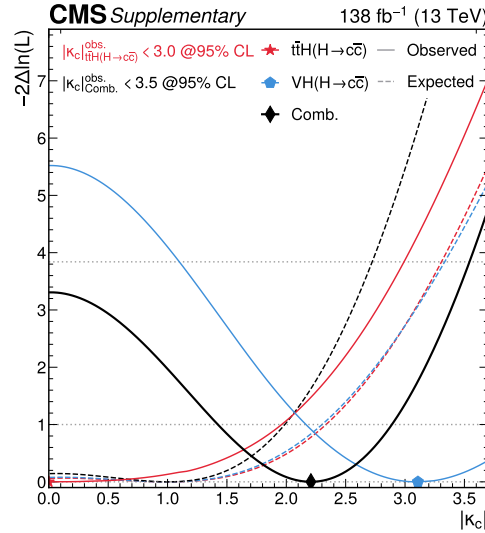


Figure B.13: Likelihood scans of κ_c with fixed $\kappa_b = 1$ in the individual $t\bar{t}H$ (red) and VH (blue) channels and their combination (black). The 68% and 95% CL intervals are indicated by the horizontal dotted lines.

surement is limited by statistical uncertainties. The observed and expected 95% CL upper limit on $\mu_{H \rightarrow c\bar{c}}$, the signal strength for the $H \rightarrow c\bar{c}$ decay channel assuming SM production rates for $t\bar{t}H$ and VH , is displayed in Fig. B.12, along with the contributions from individual analyses. Figure B.13 shows the profile likelihood scan of $|\kappa_c|$ in the combined analysis.

Figures B.14–B.16 show likelihood scans for the simultaneous fit of two parameters each, e.g., for pairs of the four signal strength parameters $\mu_{t\bar{t}H(H \rightarrow c\bar{c})}$, $\mu_{t\bar{t}H(H \rightarrow b\bar{b})}$, $\mu_{t\bar{t}Z(Z \rightarrow b\bar{b})}$, and $\mu_{t\bar{t}Z(Z \rightarrow c\bar{c})}$, and for pairs of the normalization scale factors of the $t\bar{t} + \text{jets}$ background components $t\bar{t} + \geq 2b$, $t\bar{t} + b$, $t\bar{t} + \geq 2c$, and $t\bar{t} + c$.

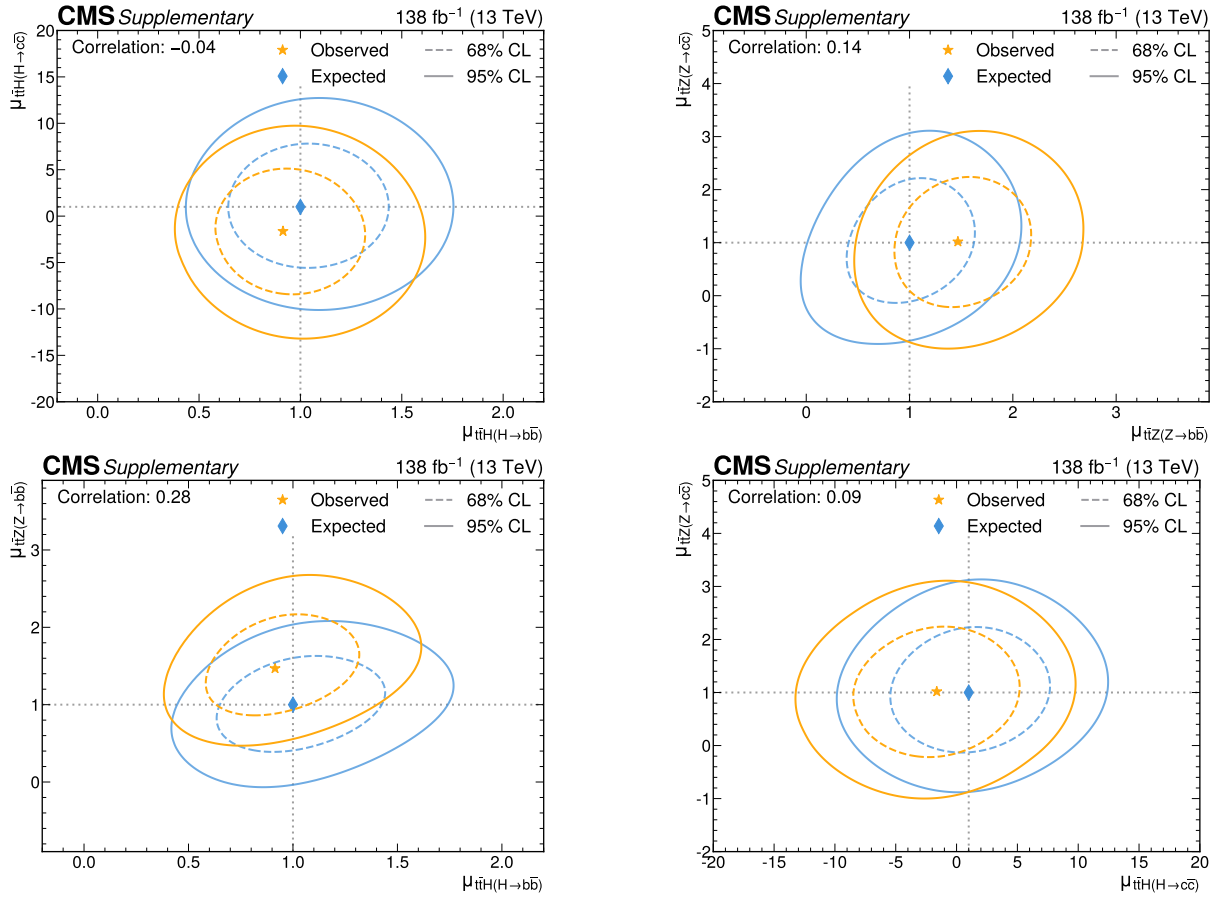


Figure B.14: Likelihood scans for the simultaneous fit of $\mu_{t\bar{t}H(H \rightarrow b\bar{b})}$ and $\mu_{t\bar{t}H(H \rightarrow c\bar{c})}$ (upper left), $\mu_{t\bar{t}Z(Z \rightarrow b\bar{b})}$ and $\mu_{t\bar{t}Z(Z \rightarrow c\bar{c})}$ (upper right), $\mu_{t\bar{t}H(H \rightarrow b\bar{b})}$ and $\mu_{t\bar{t}Z(Z \rightarrow b\bar{b})}$ (lower left), and $\mu_{t\bar{t}H(H \rightarrow c\bar{c})}$ and $\mu_{t\bar{t}Z(Z \rightarrow c\bar{c})}$ (lower right). The 68% (95%) CL intervals are indicated by the dotted (solid) lines. The observed (expected) best fit values are shown by the orange (blue) markers.

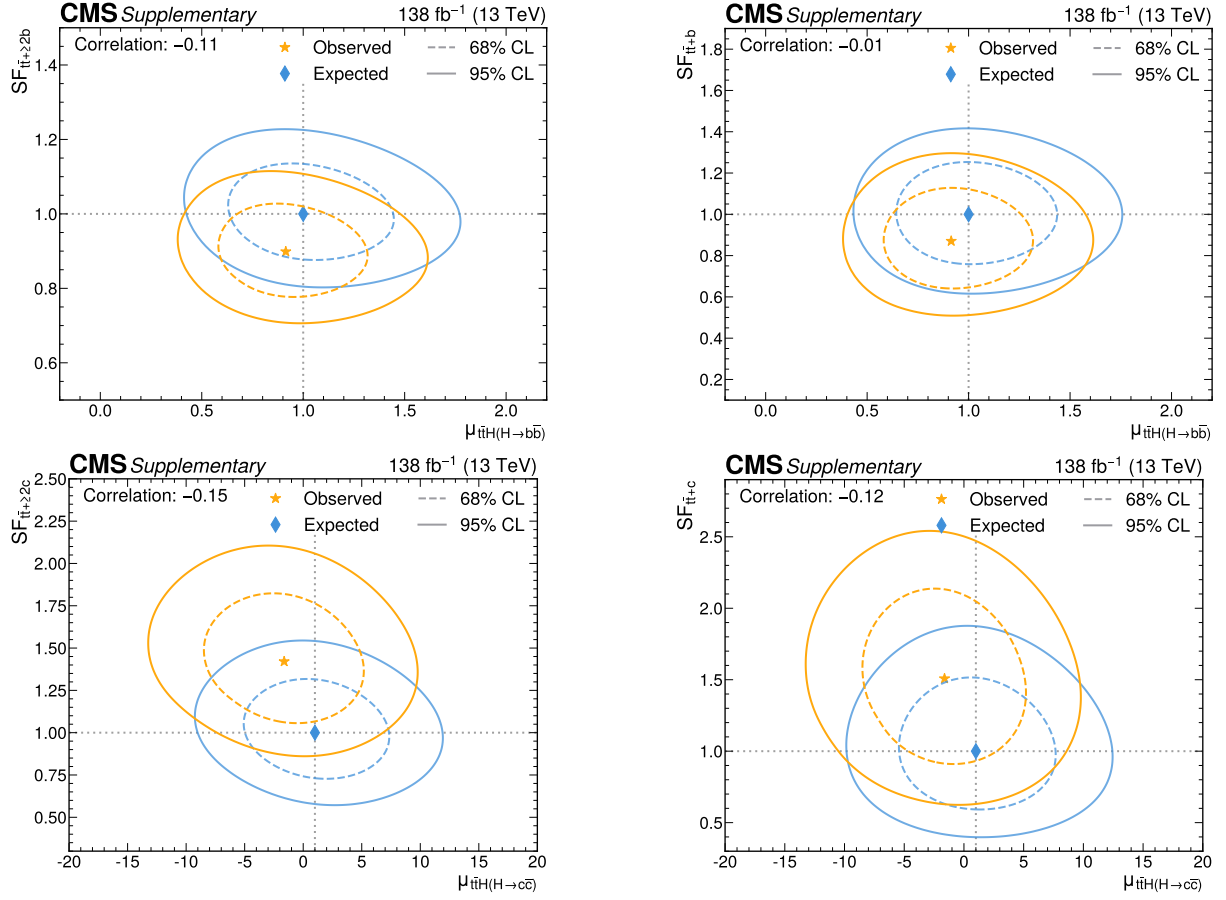


Figure B.15: Likelihood scans for the simultaneous fit of $\mu_{\text{ttH}(H \rightarrow b\bar{b})}$ and the $\text{t}\bar{\text{t}} + \geq 2\text{b}$ scale factor (upper left), $\mu_{\text{ttH}(H \rightarrow b\bar{b})}$ and the $\text{t}\bar{\text{t}} + \text{b}$ scale factor (upper right), $\mu_{\text{ttH}(H \rightarrow c\bar{c})}$ and the $\text{t}\bar{\text{t}} + \geq 2\text{c}$ scale factor (lower left), and $\mu_{\text{ttH}(H \rightarrow c\bar{c})}$ and the $\text{t}\bar{\text{t}} + \text{c}$ scale factor (lower right). The 68% (95%) CL intervals are indicated by the dotted (solid) lines. The observed (expected) best fit values are shown by the orange (blue) markers.

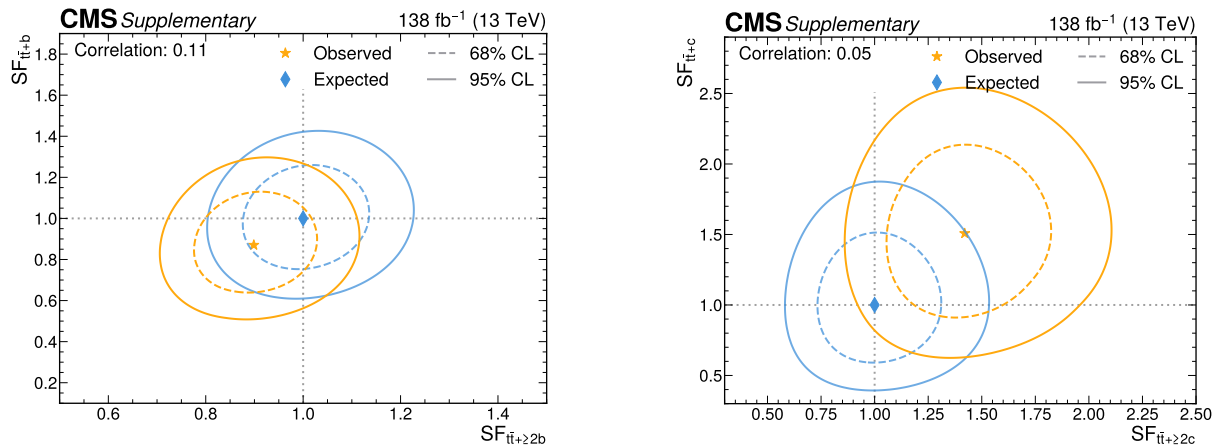


Figure B.16: Likelihood scans for the simultaneous fit of the $\text{t}\bar{\text{t}} + \geq 2\text{b}$ and $\text{t}\bar{\text{t}} + \text{b}$ scale factors (left), and of the $\text{t}\bar{\text{t}} + \geq 2\text{c}$ and $\text{t}\bar{\text{t}} + \text{c}$ scale factors (right). The 68% (95%) CL intervals are indicated by the dotted (solid) lines. The observed (expected) best fit values are shown by the orange (blue) markers.

B.10 Cross checks with alternative $t\bar{t} + \geq 1b$ background models

The robustness of the results is assessed by performing the fit for the signal strength parameters using alternative background models, focusing on variations of the $t\bar{t} + \geq 1b$ background model:

- (1) **Simple PS:** Using a simplified scheme of the PS uncertainties with only one ISR and FSR scale uncertainty instead of the 16 individual components.
- (2) **$\mu_F \times 2$:** Changing μ_F by a factor two in the $t\bar{t} + \geq 1b$ simulation and otherwise using the same $t\bar{t} + \geq 1b$ uncertainty model. This alternative μ_F and μ_R choice corresponds to the setup used in the recent measurement of $t\bar{t}H(H \rightarrow b\bar{b})$ production by the ATLAS Collaboration [98].
- (3) **$\mu_F \times 2$ & Simple PS:** As described in (2), but using the simplification of (1).
- (4) **5FS $t\bar{t} + \geq 1b$:** Using the 5FS $t\bar{t} + \geq 1b$ simulation as the nominal background model.
- (5) **5FS $t\bar{t} + \geq 1b$ & Simple PS:** As described in (4), but using the simplification of (1).

The results for the nominal fit setup as well as for variations are given in Table B.12 for the best fit signal strength parameters, the observed upper limits and the significance on the signal strengths, and in Table B.13 for the $t\bar{t} + \geq 1b$ background normalization parameters.

Table B.12: Observed signal strengths for $t\bar{t}H(H \rightarrow c\bar{c})$, $t\bar{t}H(H \rightarrow b\bar{b})$, $t\bar{t}Z(Z \rightarrow c\bar{c})$, and $t\bar{t}Z(Z \rightarrow b\bar{b})$ as obtained by the fits using alternative background models. In brackets are the observed upper limits for $t\bar{t}H(H \rightarrow c\bar{c})$ and the significance values for $t\bar{t}H(H \rightarrow b\bar{b})$, $t\bar{t}Z(Z \rightarrow c\bar{c})$, and $t\bar{t}Z(Z \rightarrow b\bar{b})$, respectively.

$t\bar{t} + \geq 1b$ bkg. model	$\mu_{t\bar{t}H(H \rightarrow c\bar{c})}$	(95% CL)	$\mu_{t\bar{t}H(H \rightarrow b\bar{b})}$	(Sign. [s.d.])	$\mu_{t\bar{t}Z(Z \rightarrow c\bar{c})}$	(Sign. [s.d.])	$\mu_{t\bar{t}Z(Z \rightarrow b\bar{b})}$	(Sign. [s.d.])
Default	-1.6 ± 4.5	(<7.8)	$0.91^{+0.26}_{-0.22}$	(4.4)	$1.02^{+0.79}_{-0.84}$	(1.2)	$1.47^{+0.45}_{-0.41}$	(3.5)
Simple PS	-0.4 ± 4.4	(<8.8)	$0.91^{+0.27}_{-0.22}$	(4.4)	$0.94^{+0.82}_{-0.73}$	(1.3)	$1.47^{+0.44}_{-0.39}$	(3.6)
$\mu_F \times 2$	$-1.7^{+4.2}_{-4.3}$	(<8.0)	$0.94^{+0.26}_{-0.23}$	(4.4)	$1.06^{+0.77}_{-0.75}$	(1.4)	$1.62^{+0.43}_{-0.38}$	(4.1)
$\mu_F \times 2$ & Simple PS	-1.0 ± 4.4	(<8.5)	$0.97^{+0.28}_{-0.23}$	(4.5)	$1.04^{+0.77}_{-0.78}$	(1.3)	$1.67^{+0.42}_{-0.37}$	(4.2)
5FS	-1.8 ± 4.3	(<7.7)	$0.97^{+0.24}_{-0.20}$	(5.7)	$1.17^{+0.77}_{-0.71}$	(1.6)	$1.14^{+0.41}_{-0.38}$	(3.0)
5FS & Simple PS	-0.9 ± 4.5	(<7.6)	$1.02^{+0.26}_{-0.21}$	(6.0)	$1.19^{+0.77}_{-0.71}$	(1.6)	$1.10^{+0.40}_{-0.37}$	(2.9)

Table B.13: Observed normalization scale factors for the background components as obtained by the fits using alternative background models. The background normalization scale factors are given for the 2L & 1L (0L) channels.

$t\bar{t} + \geq 1b$ background model	$t\bar{t} + \geq 2b$	$t\bar{t} + b$
Default	0.90 ± 0.08 (1.14 ± 0.12)	0.87 ± 0.15 (0.83 ± 0.16)
Simple PS	0.88 ± 0.07 (1.12 ± 0.11)	0.92 ± 0.16 (0.89 ± 0.18)
$\mu_F \times 2$	0.89 ± 0.06 (1.37 ± 0.10)	0.94 ± 0.17 (1.05 ± 0.21)
$\mu_F \times 2$ & Simple PS	0.90 ± 0.05 (1.41 ± 0.10)	0.95 ± 0.16 (1.06 ± 0.22)
5FS	1.54 ± 0.11 (2.06 ± 0.19)	0.91 ± 0.36 (0.62 ± 0.64)
5FS & Simple PS	1.57 ± 0.09 (2.25 ± 0.21)	0.83 ± 0.34 (0.60 ± 0.62)

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