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Combination of searches for singly produced vector-like top quarks in pp collisions at $\sqrt{s} = 13$ TeV with the ATLAS detector

The ATLAS Collaboration

A combination of searches for the single production of vector-like top quarks (T) is presented. These analyses are based on proton–proton collisions at $\sqrt{s} = 13$ TeV recorded in 2015–2018 with the ATLAS detector at the Large Hadron Collider, corresponding to an integrated luminosity of 139 fb^{-1}. The T-quark decay modes considered in this combination are into a top quark and either a Standard Model Higgs boson or a Z boson ($T \rightarrow Ht$ and $T \rightarrow Zt$). The individual searches used in the combination are differentiated by the number of leptons (e, μ) in the final state. The observed data are found to be in good agreement with the Standard Model background prediction. Interpretations are provided for a range of masses and couplings of the vector-like top quark for benchmark models and generalized representations in terms of 95% confidence level limits. For a benchmark signal prediction of a vector-like top quark SU(2) singlet with electroweak coupling, κ, of 0.5, masses below 2.1 TeV are excluded, resulting in the most restrictive limits to date.

Contents

1 Introduction

The formulation of electroweak interactions arising from a spontaneously broken gauge symmetry is a cornerstone of the Standard Model (SM). Experiments over the past four decades have confirmed this hypothesis, most notably through the precision measurements of the LEP and SLC collider programs [1, 2]. A major milestone was achieved when the ATLAS and CMS Collaborations reported the discovery [3, 4] of a new particle produced at CERN's Large Hadron Collider (LHC) possessing properties consistent with those predicted for the SM Higgs boson (H). The electroweak symmetry-breaking mechanism, where a weak-isospin doublet of fundamental scalar fields obtains a vacuum expectation value, remains the simplest hypothesis.

Following the discovery of the Higgs boson, the SM still cannot be considered a complete description of nature. For example, the theory does not explain the number of fermion generations and their mass hierarchy and mixing angles, nor the origin of the matter–antimatter asymmetry in the universe. It also does not have a viable dark matter particle. Therefore, the SM is generally regarded as a low-energy approximation of a more fundamental theory with new degrees of freedom and symmetries that would become manifest at higher energy. In fact, the SM violates a concept of naturalness [5] when extrapolated to energies above the electroweak scale. When extrapolated to the energy scale of new physics, a fine-tuning of the theory is required. The fine-tuning can be mitigated by the introduction of new interactions that cancel out the quadratic divergences in the Higgs boson mass. To this effect, several explanations are proposed in theories beyond the SM (BSM).

Proposed BSM models typically address the naturalness problem by postulating a new symmetry. For example, supersymmetry is a Bose–Fermi symmetry, and the new states related to the SM bosons and fermions by this symmetry introduce new interactions that cancel out the quadratically divergent ones [6–11]. Alternatively, the symmetry could be a spontaneously broken global symmetry of the extended theory, with the Higgs boson emerging as a pseudo-Nambu–Goldstone boson [12]. Examples of models that implement this idea are Little Higgs [13, 14] and Composite Higgs [15, 16] models. The new states realizing the enhanced symmetry are generically strongly coupled resonances of new confining dynamics. These include vector-like quarks (VLQs), defined as color-triplet spin-$1/2$ fermions whose left- and right-handed chiral components have the same transformation properties under the weak-isospin gauge group. Such quarks

Table 1: Possible VLQ multiplets allowed to mix with the SM quarks.

VLQ	(T)	(B)	$\begin{pmatrix}T\\B\end{pmatrix}$	$\begin{pmatrix}X\\T\end{pmatrix}$	$\begin{pmatrix}B\\Y\end{pmatrix}$	$\begin{pmatrix}X\\T\\B\end{pmatrix}$	$\begin{pmatrix}T\\B\\Y\end{pmatrix}$
Isospin	0	0	1/2	1/2	1/2	1	1
Hypercharge	$+2/3$	$-1/3$	$+1/6$	$+7/6$	$-5/6$	$+2/3$	$-1/3$

could mix with like-charge SM quarks [17, 18], and the mixing of the SM top quark with a charge $+2e/3$ vector-like quark (where e is the electric charge of the electron) could play a role in regulating the sensitivity to the Higgs boson mass. Hence, VLQs emerge as a characteristic feature of several non-supersymmetric models [19].

In order for VLQs to mix with the SM quarks [17, 18], some constraints are needed on their allowed quantum numbers to preserve gauge invariance. Therefore, in order to generate Yukawa terms in the Lagrangian without changing the scalar sector, only seven renormalizable possibilities [20] are allowed, which are summarized in Table 1. The vector-like T and B have electric charge $+2e/3$ and $-1e/3$, respectively. VLQs with other electric charges could also exist, such as the X and Y quarks with $+5e/3$ and $-4e/3$, respectively.

The renormalizable electroweak representations consist of (T) or (B) SU(2) singlets, (X, T), (T, B), or (B, Y) doublets and (X, T, B) or (T, B, Y) triplets. In all representations, they couple to the SM quarks via an exchange of charged $(W^{\pm})$ or neutral (Z, H) bosons. The simplified Lagrangian [21] below summarizes the interaction of the VLQ and SM quarks:

$$\mathcal{L} = \sum_{Q,q,\zeta}\left[\frac{g_W}{\sqrt{2}}\kappa_{\zeta}^{Qq}\bar{Q}\not{W}P_{\zeta}q + \frac{g_W}{2c_W}\tilde{\kappa}_{\zeta}^{Qq}\bar{Q}\not{Z}P_{\zeta}q + \hat{\kappa}_{\zeta}^{Qq}H\bar{Q}P_{\zeta}q\right] + \text{H.c.}, \tag{1}$$

where Q represents a VLQ, ζ represents the chirality with P_{ζ} being the corresponding projection operator, q represents a SM quark of up or down type, and the electroweak couplings κ_{ζ}^{Qq}, $\tilde{\kappa}_{\zeta}^{Qq}$, and $\hat{\kappa}_{\zeta}^{Qq}$ determine the coupling strengths between Q and q when mediated by the W, Z, and H bosons, respectively. The mass hierarchy of the SM quarks suggests that VLQs interact predominantly with the third-generation SM quarks [22, 23]. Hence, VLQ interactions with lighter generations are set to zero in the simplified representation of Eq. (1). Furthermore, this formulation assumes there are no additional mediators other than the W, Z, and H bosons.

In proton–proton (pp) collisions, VLQs can be produced singly via the electroweak interaction (as illustrated by the leading-order (LO) Feynman diagram in Figure 1) or in pairs via the strong interaction. While the cross-section for pair production is generally given by quantum chromodynamics, the single-production cross-section explicitly depends on the coupling of the VLQs to SM electroweak bosons. Search strategies for VLQs were outlined previously [23–27]. Results of searches for chiral fourth-generation quarks apply, though interpreting the exclusions was difficult when the quarks were assumed to decay entirely via the charged-current process. When VLQs are added to the SM, flavor-changing tree-level neutral-current decays of such new heavy quarks appear [28], while they are not present for SM quarks at tree level and are also highly suppressed at loop level by the Glashow–Iliopoulos–Maiani (GIM) mechanism [29]. Following Ref. [30], the relative couplings of VLQs to W, Z and H bosons are given in terms of the

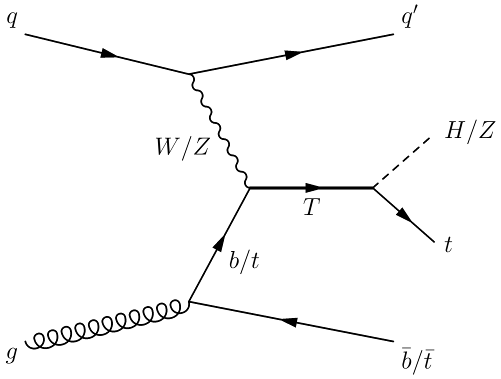

Figure 1: Illustrative leading-order Feynman diagram of single vector-like T production in association with a t or b quark and subsequent decay into either Ht or Zt.

parameters ξ_W, ξ_Z and ξ_H, respectively. In the asymptotic limit of large VLQ mass, the ξ parameters correspond to the branching ratios of the T quark decay to W, Z and H bosons. The asymptotic limit holds to good approximation for VLQ masses above 1 TeV. In the T SU(2) singlet representation, $\xi_W = 0.5$ and $\xi_Z = \xi_H = 0.25$. If the T quarks are part of an (X, T) or (T, B) SU(2) doublet then $\xi_W = 0.0$, and $\xi_Z = \xi_H = 0.5$.

Vector-like T and B quarks were searched for both at ATLAS and CMS in Run 1, and more recently with the Run 2 data. The Run 2 searches focused on VLQ pair production [31–46] and recently also on VLQ single production [32, 34, 47–59]. Searches for VLQ are summarized by the ATLAS and CMS Collaborations in Refs. [60, 61]. The most stringent limits on T- and B-quark masses come from the latest ATLAS and CMS searches. The excluded masses for VLQs depend on the branching ratio. In the case of SU(2) doublet representations (T, B) where both VLQs are considered and assumed to be mass degenerate, T quark masses below 1.6 TeV [46] are excluded at 95% confidence level (CL). When no assumption is made on the branching ratio or mass degeneracy, then T quarks with masses below 1.5 TeV [44] are excluded. In the case of SU(2) singlet representations masses below 1.5 TeV [44] are excluded. The pair production limits assume a narrow-width resonance, an assumption not made for single production. In single production, for which the interpretation of results is more challenging due to the additional coupling factor, analyses have set limits in the coupling/mixing-angle-vs.-mass plane, reaching up to nearly 2 TeV [55] for large coupling and mixing angles.

This paper describes a combination of three analyses, differentiated by the number of light leptons (e, μ) in the final state. The search regions for each analysis, including the control regions, are designed to be orthogonal as they target different decay channels. This is achieved by requiring exactly zero leptons (electrons or muons) in the "Monotop" analysis [47], exactly one lepton in the "HtZt" analysis [62], and two or more leptons in the "OSML" (Opposite-Sign Multi-Lepton) analysis [55]. All searches use the full Run 2 ATLAS dataset collected with the ATLAS detector during 2015–2018, corresponding to 139 fb^{-1} of pp collisions at $\sqrt{s} = 13$ TeV. The searches are combined taking into account correlations in the background modeling and systematic uncertainties. In the absence of a significant excess above the SM expectation, the results are used to set upper limits on the single production of T quarks for several scenarios of the mass, the universal coupling strength κ, and the relative couplings to W, Z and Higgs bosons. This is the first combination of searches for single T-quark production by the ATLAS Collaboration and the results provide the most restrictive bounds to date.

2 ATLAS detector

The ATLAS experiment [63] at the LHC is a multipurpose particle detector with a forward–backward symmetric cylindrical geometry and a near 4π coverage in solid angle.[1] It consists of an inner tracking detector surrounded by a thin superconducting solenoid providing a 2 T axial magnetic field, electromagnetic and hadronic calorimeters, and a muon spectrometer. The inner tracking detector covers the pseudorapidity range $|\eta| < 2.5$. It consists of silicon pixel, silicon microstrip, and transition radiation tracking detectors. Lead/liquid-argon (LAr) sampling calorimeters provide electromagnetic (EM) energy measurements with high granularity within the region $|\eta| < 3.2$. A steel/scintillator-tile hadronic calorimeter covers the central pseudorapidity range ($|\eta| < 1.7$). The endcap and forward regions are instrumented with LAr calorimeters for EM and hadronic energy measurements up to $|\eta| = 4.9$. The muon spectrometer surrounds the calorimeters and is based on three large superconducting air-core toroidal magnets with eight coils each. The field integral of the toroids ranges between 2.0 and 6.0 T m across most of the detector. The muon spectrometer includes a system of precision tracking chambers up to $|\eta| = 2.7$ and fast detectors for triggering up to $|\eta| = 2.4$. The luminosity is measured mainly by the LUCID–2 [64] detector, which is located close to the beampipe. A two-level trigger system is used to select events [65]. The first-level trigger is implemented in hardware and uses a subset of the detector information to accept events at a rate below 100 kHz. This is followed by a software-based trigger that reduces the accepted event rate to 1 kHz on average depending on the data-taking conditions. A software suite [66] is used in data simulation, in the reconstruction and analysis of real and simulated data, in detector operations, and in the trigger and data acquisition systems of the experiment.

3 Data and simulated event samples

This combination uses pp collision data collected with the ATLAS detector during the 2015–2018 data taking period, at a collision energy of $\sqrt{s} = 13$ TeV, corresponding to an integrated luminosity of 139 fb^{-1} [64, 67]. Only events recorded with a single-electron trigger, a single-muon trigger or a $E_{\text{T}}^{\text{miss}}$ trigger [68–70] under stable beam conditions, and for which all relevant detector subsystems were operational [71], are used in these analyses. The trigger requirements of the individual analyses can be found in the respective publications [47, 55, 62].

Monte Carlo (MC) simulated events are used to evaluate background contamination and modeling, signal acceptance, optimization of the event selection, and evaluation of systematic uncertainties. They are centrally produced with the well-established ATLAS event generation procedure [72]. For all samples, a full simulation of the ATLAS detector was performed using GEANT 4 [73]. A faster simulation, where the full GEANT 4 simulation of the calorimeter response is replaced by a detailed parameterization of the shower shapes [74], was adopted for some of the samples used to estimate systematic uncertainties.

The effect of multiple interactions in the same and neighboring bunch crossings (pile-up) was modeled by overlaying simulated hard-scattering events with inelastic pp events generated with PYTHIA8 (v8.186) [75]

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[1] ATLAS uses a right-handed coordinate system with its origin at the nominal interaction point (IP) in the center of the detector and the z-axis along the beam pipe. The x-axis points from the IP to the center of the LHC ring, and the y-axis points upwards. Polar coordinates (r, ϕ) are used in the transverse plane, ϕ being the azimuthal angle around the z-axis. The pseudorapidity is defined in terms of the polar angle θ as $\eta = -\ln\tan(\theta/2)$ and is equal to the rapidity $y = \frac{1}{2}\ln\left(\frac{E+p_z c}{E-p_z c}\right)$ in the relativistic limit. Angular distance is measured in units of $\Delta R \equiv \sqrt{(\Delta y)^2 + (\Delta\phi)^2}$.

Table 2: Overview of the nominal simulated background samples, including information about the matrix element (ME) generator and parton distribution function (PDF) set, parton shower (PS), set of tuned parameters (Tune), and higher-order cross-section used for normalization. For single top the t- and s-channel production cross-sections are calculated at next-to-NLO (NNLO) in QCD, while the Wt production cross-section is calculated at NLO and includes third-order corrections of soft-gluon emissions by resuming next-to-next-to-leading logarithm (NNLL) terms.

Process	ME event generator	ME PDF	PS and hadronization	Tune	Cross-section calculation
W/Z+jets	Sherpa 2.2.1 [78]	NNPDF3.0NNLO [80]	Sherpa [78]	Default	NNLO [86]
$t\bar{t}W/Z$	MadGraph5_aMC@NLO 2.3.3 [87]	NNPDF3.0NLO [80]	Pythia 8.2 [79]	A14	NLO
tZ	MadGraph5_aMC@NLO 2.3.3 [87]	NNPDF2.3LO [76]	Pythia 8.2 [79]	A14	NLO
tWZ	MadGraph5_aMC@NLO 2.3.3 [87]	NNPDF2.3LO [76]	Pythia 8.2 [79]	A14	NLO
$t\bar{t}$	Powheg-Box [88]	NNPDF2.3LO [76]	Pythia 8.2 [79]	A14	NNLO+NNLL [89, 90]
Single top	Powheg-Box [88]	NNPDF2.3LO [76]	Pythia 8.2 [79]	A14	NNLO/NLO+NNLL [91–95]
Multiboson	Sherpa 2.2.1–2.2.2 [78]	NNPDF3.0NNLO [80]	Sherpa	Default	NLO

using the NNPDF2.3LO parton distribution function (PDF) set [76] and the A3 set of tuned parameters (tune) [77]. The MC events were weighted to reproduce the distribution of the average number of interactions per bunch crossing ($\langle\mu\rangle$) observed in the data.

Table 2 summarizes the setups used in the simulated SM background samples. Except for the samples generated with Sherpa [78], all samples are interfaced with Pythia 8.2 [79] for the modeling of the parton shower (PS), hadronization and underlying event (UE) using the NNPDF2.3LO PDF set [80] and the A14 tune [81]. Alternative samples to study the impact of systematic uncertainties due to the PS and hadronization model are instead interfaced with Herwig 7 [82, 83] using the MMHT2014LO PDF set [84] and the H7UE tune [82]. Additional details and other uncertainties in background modeling are given in the respective references [47, 55, 62]. The EvtGen 1.6.0 [85] program was used to model b- and c-hadron decays for all samples showered using Pythia 8.2 or Herwig 7, with the exception of the $t\bar{t}V$ ($V = W, Z$) samples, where EvtGen 1.2.0 is used instead.

Samples modeling the single production of T quarks were generated using the MadGraph5_aMC@NLO program [87] at LO in quantum chromodynamics (QCD) for matrix elements (ME) with the "VLQ" Universal FeynRules Output (UFO) model [96] implementing the Buchkremer model introduced in Ref. [97] and Eq. (1). The generated events were interfaced with Pythia 8.2 using the NNPDF23LO PDF set and the A14 tune. This model uses the 4-flavor scheme and all tree-level processes are included. The VLQs are assumed to couple exclusively to SM quarks of the third generation and SM bosons. In these analyses the pair production of VLQs is not considered.

Separate samples were produced for the $T(\rightarrow Ht)qb$, $T(\rightarrow Zt)qb$, $T(\rightarrow Ht)qt$ and $T(\rightarrow Zt)qt$ processes. Samples were generated with a 200 GeV spacing for $T(\rightarrow Ht)qb$ and $T(\rightarrow Zt)qb$ processes, and ME-based weights were used to reweight the samples to intermediate mass points to create 100 GeV intervals in the mass grid. Since the relative variations in the resonance lineshape of $T(\rightarrow Ht)qt$ and $T(\rightarrow Zt)qt$ samples are larger as a function of the T quark mass, the reweighting requires additional mass points for the precision desired, and samples for these processes were generated with 100 GeV mass spacing.

For similar reasons, the universal coupling between the T quark and the gauge boson, κ, was set to a value of 1.0 for the $T(\rightarrow Ht)qb$ and $T(\rightarrow Zt)qb$ samples, and reweighted to other values of κ down to a value of 0.1, while this reweighting for the $T(\rightarrow Ht)qt$ and $T(\rightarrow Zt)qt$ samples is only valid within much narrower ranges of κ. Thus, for the latter two processes, samples were produced at κ values of 0.2, 0.4, 0.7 and 1.0, and used to reweight to neighboring coupling values.

Table 3: Summary of the target signal and decay channels for the three analyses included in the combination and the discriminating variables used.

Analysis	Target signal	Decay channels	Discriminants
MONOTOP	$Wb/Zt \to T \to Zt$	$Zt \to \nu\nu bqq$ (0ℓ)	BDT score
HTZT	$Wb/Zt \to T \to Ht/Zt$	$Ht/Zt \to bbb\ell\nu/qqb\ell\nu$ (1ℓ)	m_{eff}
OSML	$Wb/Zt \to T \to Zt$	$Zt \to \ell\ell b\ell\nu$ (3ℓ), $Zt \to \ell\ell bqq$ (2ℓ)	Z boson p_{T}

Benchmark samples with specific values of the relative coupling parameters $\vec{\xi}$ (where $\vec{\xi} = (\xi_W, \xi_Z, \xi_H) = (0.50, 0.25, 0.25)$ for SU(2) singlets in the high-mass asymptotic limit)[2] were constructed by combining the samples for individual production and decay modes by their appropriate relative proportions. The samples were normalized by multiplying the LO cross-section times branching ratio for given assumed couplings by a correction factor to account for finite width effects [30, 98], and by next-to-leading-order (NLO) k-factors computed in the narrow-width approximation [99]. A change in the dynamic scale in MADGRAPH at the T-quark width-over-mass threshold $\Gamma_{\text{T}}/m_{\text{T}} = 0.1$, leads to a discontinuity in the computed cross-section [98]. As a result, two different parameterizations of the cross-section are available: $\sigma_{\text{low}}(\Gamma_{\text{T}}/m_{\text{T}})$ for the $\Gamma_{\text{T}}/m_{\text{T}} < 0.1$ regime, and $\sigma_{\text{high}}(\Gamma_{\text{T}}/m_{\text{T}})$ for $\Gamma_{\text{T}}/m_{\text{T}} > 0.1$. An averaging procedure is used to obtain a smooth cross-section $\sigma(\Gamma/M)$ across the mass and coupling grid:

$$\sigma(\Gamma_{\text{T}}/m_{\text{T}}) = \begin{cases} \sigma_{\text{low}}(\Gamma_{\text{T}}/m_{\text{T}}) + \frac{1}{2}[\sigma_{\text{high}}(0.1) - \sigma_{\text{low}}(0.1)], & \text{if } \Gamma_{\text{T}}/m_{\text{T}} < 0.1 \\ \sigma_{\text{high}}(\Gamma_{\text{T}}/m_{\text{T}}) - \frac{1}{2}[\sigma_{\text{high}}(0.1) - \sigma_{\text{low}}(0.1)], & \text{if } \Gamma_{\text{T}}/m_{\text{T}} \geq 0.1. \end{cases}$$

An additional uncertainty of $\frac{1}{2}[\sigma_{\text{high}}(0.1) - \sigma_{\text{low}}(0.1)]$ is assigned on the cross-section at every point to account for this choice.

4 Description of input analyses

The analyses search for the production of charged $+2e/3$ vector-like T quarks that decay into a H boson and a top quark ($T \to Ht$) or a Z boson and a top quark ($T \to Zt$). The targeted vector-like T production topology is displayed in Figure 1. Four production and decay modes are possible: $Wb \to T \to Ht$, $Wb \to T \to Zt$, $Zt \to T \to Ht$ and $Zt \to T \to Zt$. The final state is characterized by the presence of multiple (b-tagged) jets due to the SM quarks and bosons produced, along with the recoiling initial-state quark which typically manifests as a forward jet. Due to the difference between the masses of the top and bottom quarks, b-associated (or W-mediated) T-quark production is kinematically favored over t-associated (or Z-mediated) production. However, in certain gauge representations, such as with a (T, B) or an (X, T) SU(2) doublet, the coupling to W bosons vanishes, and the t-associated mode is the only allowed production channel.

Full descriptions of the event selection for the different analyses are available in Refs. [47, 55, 62]. A summary of the target signals, decay channels and discriminants of each analysis is given in Table 3.

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[2] The parameterization of VLQ Lagrangian in terms of the κ and $\vec{\xi}$ parameters was introduced in Ref. [30] and is used for the interpretation presented. The conversion to the coupling convention in Eq. (1) is obtained through a one-to-one mapping of the tree-level couplings in the Lagrangian. The ξ_W, ξ_Z, ξ_H parameters satisfy the constraint $\xi_W + \xi_Z + \xi_H = 1$ and represent the branching ratios of T decaying into Wb, Zt, and Ht in the narrow-width approximation.

Common features include the requirement of significant energy (or missing transverse momentum) observed in the detector as leptons (electrons or muons) and jets. Jets are reconstructed by applying the anti-k_t algorithm [100, 101] to topological calorimeter-energy clusters and charged-particle tracks processed with a particle-flow algorithm [102] with fixed radius parameters of $R = 0.4$ (small-radius jets) and $R = 1.0$ (large-radius jets), and with a variable-radius parameter [103] optimized for top-quark tagging. Small-radius jets may be central ($|\eta| < 2.5$) or forward ($2.5 < |\eta| < 4.5$). Central jets may be b-tagged, while forward jets are a distinctive signature of singly produced T quarks, where the jet scatters off of a vector boson from one of the incoming partons. By design, these analyses have orthogonal selections. This is achieved by requiring exactly zero leptons in the MONOTOP analysis, exactly one lepton in the HTZT analysis, and two or more leptons in the OSML analysis. As a result, there are no overlapping events in the signal regions.

The MONOTOP analysis [47] focuses on events with a reconstructed boosted hadronically-decaying top quark produced in association with large missing transverse momentum and a forward jet. The output score of a Boosted Decision Tree (BDT) algorithm is used in the definition of the signal, control and validation regions, and is the discriminating variable in the signal regions.

The HTZT search [62] analyzes data with final states containing a single lepton with multiple jets including b-jets and a forward jet. The presence of boosted heavy resonances in the event is exploited to discriminate the signal from the SM background. Due to the strong signal discrimination power, the “effective mass,” m_{eff}, defined as the scalar sum of the transverse momentum (p_{T}) of all central small-radius jets and leptons in the event and the missing transverse energy, $E_{\mathrm{T}}^{\mathrm{miss}}$, is chosen as the observable. The analysis is split into five signal regions based on jet multiplicity to further enhance the sensitivity.

The final state of the OSML analysis [55] is characterized by the presence of a pair of electrons or muons with opposite-sign charges that forms a reconstructed Z boson candidate, and by the presence of b-tagged jets and a forward jet. Events with exactly two or at least three leptons are categorized into two independently optimized analysis channels. The transverse momentum of the Z boson is chosen as the observable due to its discriminating power.

5 Statistical analysis and systematic uncertainties

For each benchmark scenario considered in this search, the distributions of the discriminating variables of each analysis across their respective search regions are jointly analyzed to test for the presence of signal. A combined likelihood function is constructed as a product of Poisson probability terms over all bins considered in each analysis. Systematic uncertainties are implemented as nuisance parameters with constraints described by Gaussian distributions.

The three analyses take different approaches to model their respective backgrounds with different associated systematic uncertainties. Although they explore significantly different phase spaces, $t\bar{t}$ (and $t\bar{t}V$), Z+jets and diboson production dominate the background in the signal regions. Each analysis applies a different background treatment, and as the specific background contributions vary, the normalization factors are also determined independently. As a result, uncertainties in the theoretical modeling and normalization of the background processes in each of the analyses are assumed to be uncorrelated.

Detector-related uncertainties are applied, including those pertaining to the lepton measurement and identification, missing transverse momentum measurement, and jet-related quantities. These uncertainties are applied to both signal and background samples and are correlated where similar selection criteria are used (see Table 4). Furthermore, each of the analyses employs b-tagging to enhance the signal separation. In the Monotop and Osml analyses, the b-tagging implementation is identical and the associated systematic uncertainties are correlated. The HtZt analysis uses track-based jets instead of calorimeter-based jets and therefore the systematic uncertainties are left uncorrelated between this channel and the other two. In practice the choice of decorrelating this channel is observed to have no impact on the result.

Similar to the b-tagging uncertainties, jet-related systematic uncertainties are considered to be correlated only between analyses that use the same jet definition. There are three exceptions. First, the jet energy resolution (JER) uncertainty is decorrelated between the Monotop analysis and the others, as the former uses an alternative scheme for this uncertainty. Although this is a conservative choice, in practice it is observed to have no impact on the result due to the insensitivity of the analyses to these jet uncertainties. Second, the jet energy scale (JES) uncertainties for small-radius jets and large-radius jets are partially correlated. This is implemented via a set of nuisance parameters, a subset of which are common to both types of jets, while other nuisance parameters in the set apply only to one of the two types of jets. Third, the jet mass resolution (JMR) uncertainties are uncorrelated between the HtZt and Monotop analyses (and are not present in the Osml analysis). The Monotop analysis uses JMR uncertainties related to large-radius jets, while the HtZt analysis uses JMR uncertainties related to small-radius jets.

Detector uncertainties affecting the signal acceptance are considered when setting exclusion limits, but those affecting the production cross-section or signal shape are not. However, the uncertainty in the theoretical signal cross-section prediction (Section 3) is shown in Figures 2 and 3.

Uncertainties due to the limited size of the simulated samples are taken into account with dedicated parameters in the fit that are independent across the bins. These parameters are included with Poisson constraints. Finally, a set of unconstrained parameters are included to control the normalization of certain background processes in each analysis. Table 4 summarizes the systematic uncertainty model used in the fit.

The likelihood function depends on the signal-strength parameter μ, which multiplies the predicted production cross-section for signal, and θ, the set of nuisance parameters that encode the effect of systematic uncertainties in the signal and background expectations. Therefore, the expected total number of events in a given bin depends on μ and θ.

The test statistic q_μ is defined as the profile likelihood ratio: $q_\mu = -2\ln(\mathcal{L}(\mu, \hat{\hat{\theta}}_\mu)/\mathcal{L}(\hat{\mu}, \hat{\theta}))$. Here, $\hat{\mu}$ and $\hat{\theta}$ are the values of the parameters μ and θ that simultaneously maximize the likelihood function $\mathcal{L}(\mu, \theta)$ (subject to the constraint $0 \leq \hat{\mu} \leq \mu$), whereas $\hat{\hat{\theta}}_\mu$ are the values of the nuisance parameters that maximize the likelihood function for a given value of μ. The statistic used for the discovery test, to compute the compatibility of the observed data with the the background-only hypothesis, is obtained by setting $\mu = 0$ in the profile likelihood ratio and leaving $\hat{\mu}$ unconstrained: $q_0 = -2\ln(\mathcal{L}(0, \hat{\hat{\theta}}_0)/\mathcal{L}(\hat{\mu}, \hat{\theta}))$. The p-value of the discovery test is given by the integral of the probability distribution of q_0 above the observed q_0 value when assuming the background-only hypothesis, and it is computed using the asymptotic approximation detailed in Ref. [104]. For each signal scenario considered, the upper limit on the signal production cross-section is computed using q_μ in the $\mathrm{CL_s}$ method [105, 106], also in the asymptotic approximation. For a given signal scenario, values of the production cross-section (parameterized by μ) yielding $\mathrm{CL_s} < 0.05$ are excluded at $\geq 95\%$ CL. The combination is performed with RooStats [107] with statistical models implemented using RooFit [108] and HistFactory [109].

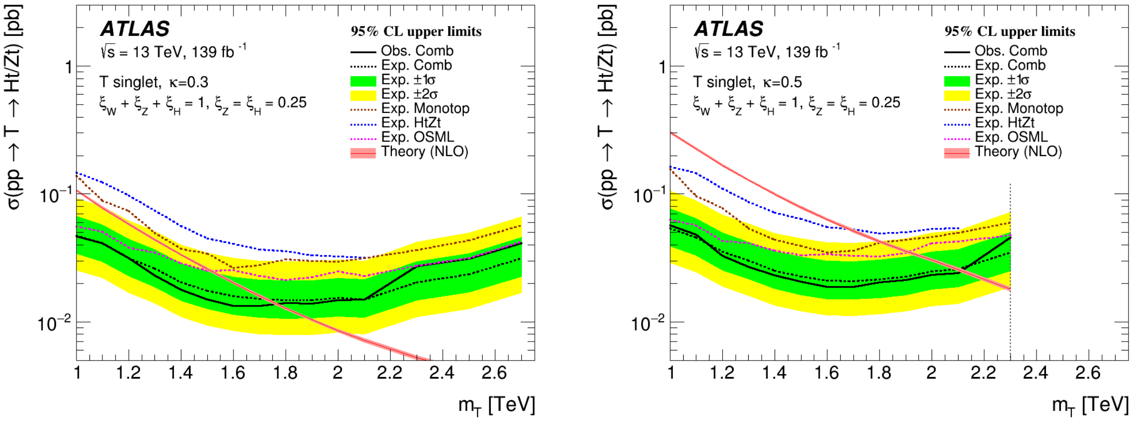
Table 4: Summary of systematic uncertainties and normalization factors included in the combined likelihood fit. A ✓indicates the uncertainty is included in a specific channel. The normalization of the largest backgrounds in the HtZt analysis are constrained with nuisance parameters subject to Gaussian constraints.

Category	Monotop	HtZt	OsML	Correlating
		Lepton and $E_{\mathrm{T}}^{\mathrm{miss}}$ uncertainties		
Electron uncertainties		✓	✓	All
Muon uncertainties		✓	✓	All
$E_{\mathrm{T}}^{\mathrm{miss}}$ uncertainties	✓	✓	✓	All
		Jet uncertainties		
JES uncertainties	✓	✓	✓	All
JER uncertainties	✓	✓	✓	HtZt and OsML
JMS uncertainties		✓		None
JMR uncertainties	✓	✓		None
		Tagging uncertainties		
Flavor-tagging uncertainties	✓	✓	✓	Monotop and OsML
Top-tagging uncertainties	✓			None
W/Z-tagging uncertainties	✓			None
Background modeling uncertainties (constrained)	✓	✓	✓	None
		Background normalization factors (unconstrained)		
$t\bar{t}$ normalization	✓			None
V+jets normalization	✓			None
Z+light-jets normalization			✓	None
Z+heavy-flavor normalization			✓	None
$t\bar{t}V$ normalization			✓	None
VV normalization			✓	None

6 Results

No significant excess above the SM expectations are observed in any of the analysis channels considered for the combination. A signal search is performed using the combined analyses and no significant excess is found. Scanning across the m_{T} and κ parameters, the most significant local p_0-value of 0.14 (0.10) for the SU(2) singlet (doublet) interpretation is found for the signal point m_{T} = 2.1 TeV and κ = 0.1. Good agreement with SM predictions is also found in the combined background-only fit to data. Therefore, upper limits on the cross-section are set at 95% CL as a function of m_{T} and κ. The limits are calculated for the sum of the production cross-sections times branching ratio of the four production and decay modes considered and denoted as $\sigma(pp \to T \to Zt/Ht)$. In contrast, the OsML and Monotop analyses were not designed to be sensitive to the $T \to Ht$ decay mode, and thus the corresponding publications reported upper limits on a subset of the processes ($T \to Zt$).

By comparing the obtained cross-section limits with the theoretical cross-section, limits are derived on m_{T} and κ. As the signal efficiencies for the considered signal modes are generally different, limits are independently determined for combinations of m_{T}, κ, and branching ratios. Motivated by the Goldstone equivalence theorem [110], which states that the branching ratios of T quark decaying into Zt and Ht become similar in the large-m_{T} limit under the narrow-width approximation, $\xi_Z = \xi_H$ is required.



(a) (b)

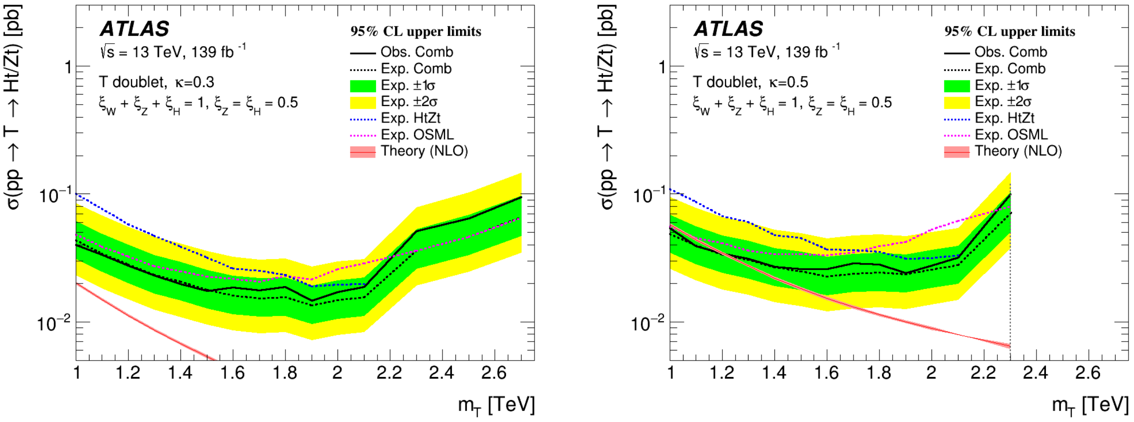
Figure 2: Observed (solid line) and expected (dashed line) 95% CL upper limits on the total cross-section $\sigma(pp \rightarrow T \rightarrow Ht/Zt)$ as a function of T-quark mass in the SU(2) singlet representation assuming (a) $\kappa = 0.3$ and (b) $\kappa = 0.5$. The surrounding shaded bands correspond to 1 and 2 standard deviations around the expected limit. A vertical dashed line is drawn to indicate the lower edge of the region with $\Gamma_\mathrm{T}/m_\mathrm{T} > 50\%$ for which the theoretical calculations are no longer valid. The expected limits for the individual analyses are shown. The HtZt analysis is only included in the limit calculation for $m_\mathrm{T} < 2.1$ TeV. The red line shows the NLO theoretical cross-section prediction, with the surrounding shaded band representing the corresponding uncertainty.

The expected and observed limits on the $T \rightarrow Ht/Zt$ cross-section from the combination are presented for several illustrative benchmark points for the SU(2) singlet (with a branching ratio $T \rightarrow Wb$ of 0.5) and doublet (with a branching ratio $T \rightarrow Wb$ of 0.0) representations. Figure 2 (Figure 3) shows the limits on the total cross-section of the sum of the production and decay processes for the SU(2) singlet (doublet) representation assuming $\kappa = 0.3, 0.5$.

Following Ref. [111], this interpretation is only used where $\Gamma_\mathrm{T}/m_\mathrm{T}$ is smaller than 50%, the region in which the correction factors for the finite-width approximation and the non-resonant contributions [30, 98] are also valid. In Figure 2 and Figure 3 a vertical dashed line is drawn to indicate the lower edge of the region with $\Gamma_\mathrm{T}/m_\mathrm{T} > 50\%$. Such lower edge extends to lower mass values as the κ value increases. As a result, the highest mass for which the limit is shown decreases as the value of κ increases.

Results from the individual channels are overlaid on the combined results for comparison. The statistical combination improves the limits over the individual results for all masses and couplings. Existing limits from searches for VLQ pair production exclude T-quark masses less than 1.5 TeV, with the assumption of narrow-width resonances. These analyses do not consider pair production signals. For the SU(2) doublet representation, the combination also includes the Monotop analysis, although its contribution is negligible. For this reason, Figure 3 shows the limits from the Osml and HtZt analyses only. In both Figures 3 and 2 the HtZt analysis is included in the combination for $m_\mathrm{T} < 2.1$ TeV, for consistency with the existing analysis.

The complementarity of the different analysis channels is also evident in Figures 2 and 3. For example, the Osml analysis is most sensitive at low masses, while the sensitivity of the HtZt analysis can be seen to improve at higher masses. This is especially true in the SU(2) doublet representation, as the HtZt analysis includes signal regions that are specifically designed to target Z-mediated production processes. The experimental sensitivity of the individual channels and the combination depends on both the mass and



(a)

(b)

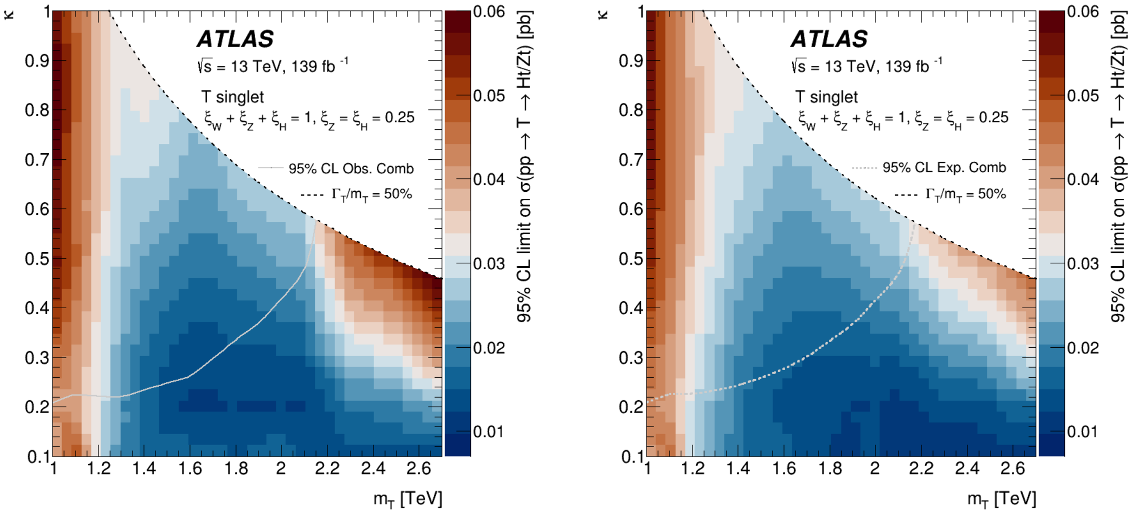
Figure 3: Observed (solid line) and expected (dashed line) 95% CL upper limits on the total cross-section $\sigma(pp \to T \to Ht/Zt)$ as a function of T-quark mass in the SU(2) doublet representation assuming (a) $\kappa = 0.3$ and (b) $\kappa = 0.5$. The surrounding shaded bands correspond to 1 and 2 standard deviations around the expected limit. A vertical dashed line is drawn to indicate the lower edge of the region with $\Gamma_\mathrm{T}/m_\mathrm{T} > 50\%$ for which the theoretical calculations are no longer valid. The expected limits for HtZt and Osml analyses are shown; the Monotop analysis is not shown due to substantially less sensitivity in this scenario. However, the Monotop analysis is included in the combined limit calculation. The HtZt analysis is only included in the limit calculation for $m_\mathrm{T} < 2.1$ TeV. The red line shows the NLO theoretical cross-section prediction, with the surrounding shaded band representing the corresponding uncertainty.

width of the T quark. In the Osml analysis, the mass dependence is clear, with the limit degrading above 2.1 TeV. This is due to the choice of binning of the discriminant (the reconstructed Z boson p_T), which was optimized to search for T quarks with masses less than 2.0 TeV. On the other hand, all three analyses use discriminants that are relatively agnostic to the resonance width (e.g., the m_eff variable for the HtZt analysis, and the reconstructed Z boson p_T in the Osml analysis). Thus, the excluded cross-section does not strongly depend on $\Gamma_\mathrm{T}/m_\mathrm{T}$ for the κ values shown in Figures 2 and 3.

The combination increases the sensitivity to a wider range of model parameters (generalized as the coupling κ) beyond the existing analyses. The cross-section limits calculated for different choices of coupling are interpreted as exclusion limits computed as a function of m_T and κ. Figure 4 (Figure 5) shows the observed and expected limits on the total cross-section for the SU(2) singlet (doublet) representation. The limits are obtained for points on the m_T–κ grid, spaced by 100 GeV in mass, and by 0.1 in κ. All three channels are combined for masses up to 2.1 TeV.

As a function of m_T and κ, Figure 4 and Figure 5 show the exclusion in a dashed line, where the region above and to the left (toward lower masses and larger couplings) is excluded. Figure 6 shows the excluded regions in the m_T–κ plane in more detail. The limits are computed for a finite number of points in the m_T–κ plane. As a result, the limits are interpolated using a piecewise function [112] between the measured points to obtain a continuous shape for the exclusion contours on the m_T–κ plane. The exclusion contours are shown both for the combination and for the individual channels. Also shown in Figure 6 are the isolines corresponding to different values of $\Gamma_\mathrm{T}/m_\mathrm{T}$. Limits are only shown for the parameter range where $\Gamma_\mathrm{T}/m_\mathrm{T} < 50\%$, where the theory calculations are known to be valid.

The combination of the three searches significantly improves the exclusion limits from the individual



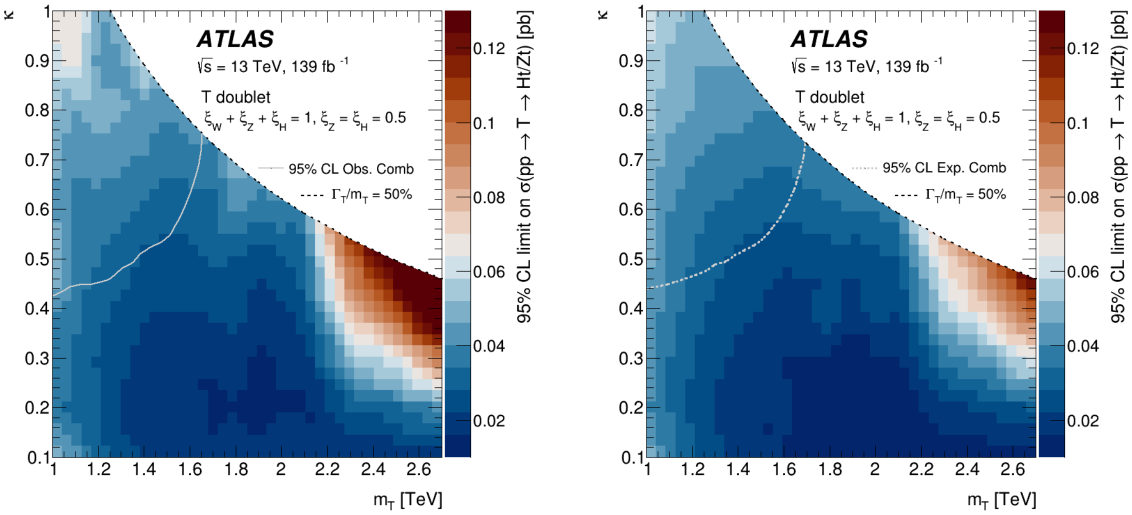
(a) (b)

Figure 4: (a) Observed and (b) expected 95% CL exclusion limits on the total cross-section $\sigma(pp \rightarrow T \rightarrow Ht/Zt)$ as a function of the universal coupling constant κ and the T-quark mass in the SU(2) singlet representation. All values of κ above the white contour line are excluded at each mass point. Limits are only presented in the regime $\Gamma_\mathrm{T}/m_\mathrm{T} < 50\%$, where the theory calculations are known to be valid.

channels. In the SU(2) singlet representation, the coupling parameter κ is constrained to be below 0.2 for the lower masses, and the mass is excluded up to 2.1 TeV for κ values near 0.6. The cross-section of a singly-produced T quark is constrained to be below 18 fb for masses in the range of 1.4–2.2 TeV and $\kappa = 0.3$ for the SU(2) singlet representation. Similarly, for the SU(2) doublet representation the coupling parameter κ is constrained to be below 0.4 for the lower masses, and the mass is excluded up to 1.7 TeV for κ values near 0.7. The cross-section of a singly-produced T quark is constrained to be below 20 fb for masses in the range of 1.4–2.1 TeV and $\kappa = 0.3$ in the SU(2) doublet representation. In both the SU(2) singlet and doublet representations, the observed cross-section limits are slightly higher than the expected cross-section limits for $\kappa = 0.3$ and $\kappa = 0.5$ for $m_\mathrm{T} > 2.2$ TeV.

The exclusion limits shown can be generalized for arbitrary values of the ξ_W parameter. Figure 7 shows the observed and expected exclusions on the T quark mass across the plane spanned by ξ_W and $\Gamma_\mathrm{T}/m_\mathrm{T}$. The relative width $\Gamma_\mathrm{T}/m_\mathrm{T}$ of the T quark is completely determined by the m_T and κ parameters. The results are shown under the theoretically motivated assumption ξ_Z=ξ_H.

As expected from the previous results, the combination improves the exclusion limits from the individual channels. The largest excluded mass is 2.1 TeV for large $\Gamma_\mathrm{T}/m_\mathrm{T}$ and $\xi_W = 0.5$. This is equivalent to the SU(2) singlet representation, with a branching ratio to Wb of 50%. The lowest excluded masses are observed for small $\Gamma_\mathrm{T}/m_\mathrm{T}$ (lower cross-section) near $\xi_W = 0.0$ and $\xi_W = 1.0$. As ξ_W apporaches 0.0, the T quark only decays into Zt and Ht, while as ξ_W approaches 1.0 there is no decay to either Zt or Ht. The overview of benchmark mass limits are shown in Table 5.



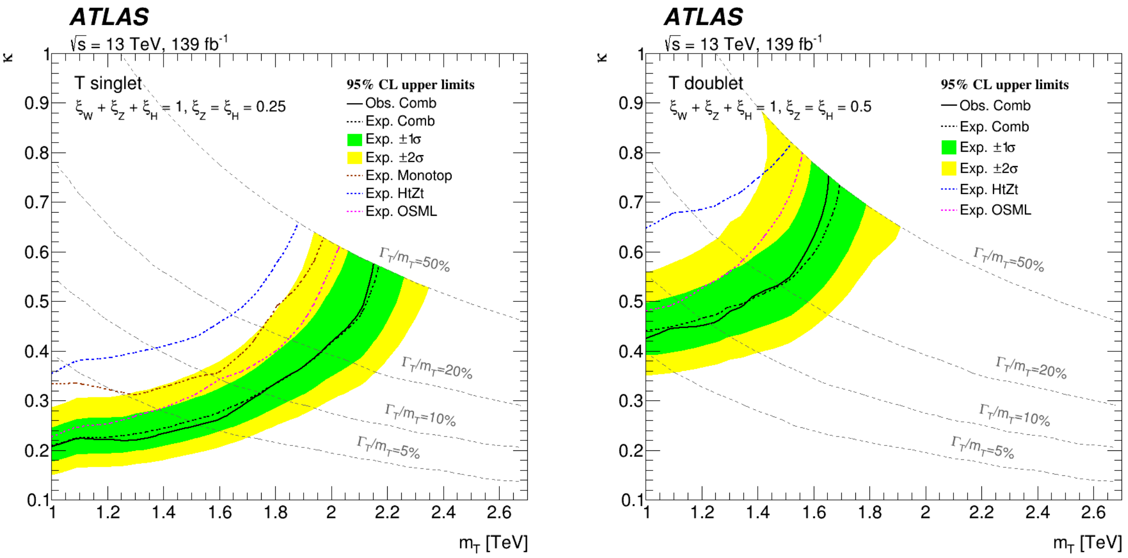
(a)

(b)

Figure 5: (a) Observed and (b) expected 95% CL exclusion limits on the total cross-section $\sigma(pp \to T \to Ht/Zt)$ as a function of the universal coupling constant κ and the T quark mass in the SU(2) doublet representation. All values of κ above the white contour line are excluded at each mass point. Limits are only presented in the regime $\Gamma_T/m_T < 50\%$, where the theory calculations are known to be valid.

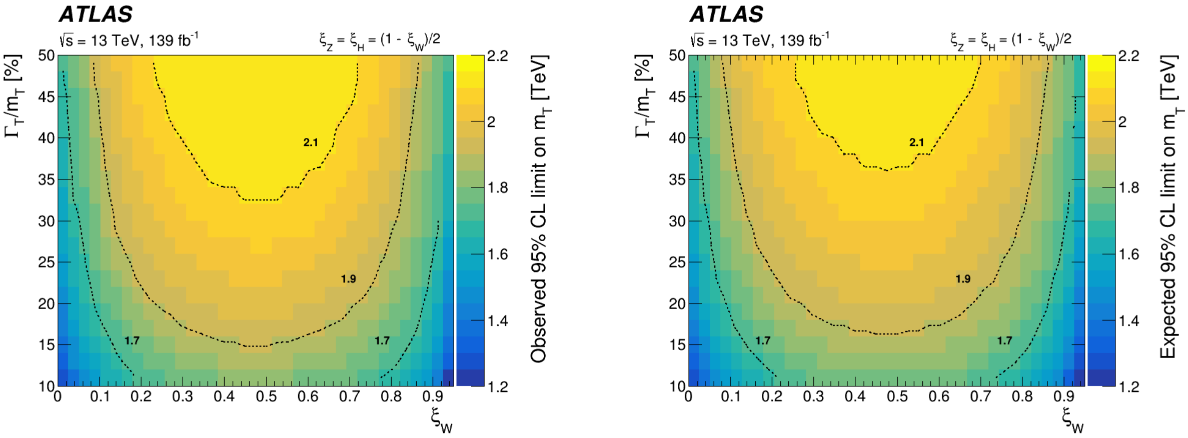
Table 5: Summary of mass limits for SU(2) singlet and doublet representations with varying Γ_T/m_T ratios. Both observed (Obs.) and expected (Exp.) limits are presented.

Representation	Γ_T/m_T [%]	Obs./Exp. mass limit [TeV]
SU(2) singlet ($\xi_W = 0.5$)	20	2.0 / 2.0
SU(2) singlet ($\xi_W = 0.5$)	50	2.1 / 2.1
SU(2) doublet ($\xi_W = 0.0$)	20	1.4 / 1.4
SU(2) doublet ($\xi_W = 0.0$)	50	1.6 / 1.7



(a) (b)

Figure 6: Observed (solid line) and expected (dashed line) 95% CL exclusion limits on the universal coupling constant κ as a function of the T quark mass in the (a) SU(2) singlet and (b) SU(2) doublet representations for the combination. All values of κ above the black contour lines are excluded at each mass point. The shaded bands correspond to 1 and 2 standard deviations around the expected limit. Also shown are the expected limits for the individual analyses. The gray dashed lines represent configurations of (m_T, κ) resulting in equal values of the relative resonance width $\Gamma_\mathrm{T}/m_\mathrm{T}$. Limits are only presented in the regime $\Gamma_\mathrm{T}/m_\mathrm{T} < 50\%$, where the theory calculations are known to be valid.



(a) (b)

Figure 7: (a) Observed and (b) expected upper limits at 95% CL on the T-quark mass as a function of the relative resonance width $(\Gamma_\mathrm{T}/m_\mathrm{T})$ and the relative coupling parameter ξ_W, for the assumption $\xi_Z = \xi_W$. The values $\xi_W = 0.5$ and $\xi_W = 0.0$ correspond to the SU(2) singlet and SU(2) doublet representations, respectively. The dashed contour lines denote exclusion limits of equal mass in units of TeV.

7 Conclusions

The first combination of results from the ATLAS Collaboration of searches for the single production of vector-like top quarks (T) decaying into Ht or Zt in hadronic and semileptonic final states has been presented. Data from pp collisions at $\sqrt{s} = 13$ TeV collected with the ATLAS detector at the LHC during 2015-2018 were used. The data corresponds to an integrated luminosity of 139 fb^{-1}. The observed data are consistent with the background prediction of the SM. Without a significant excess above the SM expectation, upper limits at 95% CL are provided for a range of masses and couplings of the vector-like top quark, based on benchmark models and generalized representations. Additionally, the exclusion limits as a function of mass (m_{T}), coupling (κ), relative width ($\Gamma_{\mathrm{T}}/m_{\mathrm{T}}$) and branching ratio are provided.

The 95% CL limits on the cross-section for T-quark production in the SU(2) singlet representation are less than 47 fb (57 fb) for all m_{T} between 1.0 and 2.7 (2.3) TeV for coupling $\kappa = 0.3$ (0.5), with a limit of 13 fb for $\kappa = 0.3$ and $m_{\mathrm{T}} = 1.6$ TeV. In the SU(2) doublet representation, the 95% CL limits on the cross-section are less than 95 fb (100 pb) over the same mass region and coupling values, with a limit of 15 fb for $\kappa = 0.3$ and $m_{\mathrm{T}} = 1.9$ TeV. The combined results improves the cross-section limits over the individual analysis limits by a factor of two in some cases. In the SU(2) singlet (doublet) representation, T-quark production is entirely excluded for $\kappa > 0.57$ (0.72), with the requirement that $\Gamma_{\mathrm{T}}/m_{\mathrm{T}} < 50\%$. For $\Gamma_{\mathrm{T}}/m_{\mathrm{T}} < 5\%$, SU(2) singlet T-quark production is excluded for $m_{\mathrm{T}} < 1.5$ TeV and $\kappa < 0.25$.

In the benchmark scenario of SU(2) singlet T-quark production with $\Gamma_{\mathrm{T}}/m_{\mathrm{T}} = 20\%$, masses less than 2.0 TeV are excluded at the 95% CL, while in the SU(2) doublet representation with $\Gamma_{\mathrm{T}}/m_{\mathrm{T}} = 20\%$ masses less than 1.4 TeV are excluded. The highest excluded mass is found for the SU(2) singlet representation assuming $\Gamma_{\mathrm{T}}/m_{\mathrm{T}} = 50\%$, where masses up to 2.1 TeV are excluded. This significantly surpasses the reach of the individual searches. These results provide the most restrictive limits on the single production of T quarks to date.

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