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The evolution of the mass–metallicity relation and its scatter in IllustrisTNG

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ABSTRACT

The coevolution of galaxies and their metal content serves as an important test for galaxy feedback models. We analyse the distribution and evolution of metals within the IllustrisTNG simulation suite with a focus on the gas-phase mass–metallicity relation (MZR). We find that the IllustrisTNG model broadly reproduces the slope and normalization evolution of the MZR across the redshift range $0 < z < 2$ and mass range $10^9 < M_*/M_\odot < 10^{10.5}$. We make predictions for the high-redshift ($2 < z < 10$) metal content of galaxies which is described by a gradual decline in the normalization of the metallicity with an average high-redshift ($z > 2$) evolution fit by $d \log(Z)/dz \approx -0.064$. Our simulations indicate that the metal retention efficiency of the interstellar medium (ISM) is low: a majority of gas-phase metals (~ 85 per cent at $z = 0$) live outside of the ISM, either in an extended gas disc, the circumgalactic medium, or outside the halo. Nevertheless, the redshift evolution in the simulated MZR normalization is driven by the higher gas fractions of high-redshift galaxies, not by changes to the metal retention efficiency. The scatter in the simulated MZR contains a clear correlation with the gas-mass or star formation rate of the system, in agreement with the observed fundamental metallicity relation. The scatter in the MZR is driven by a competition between periods of enrichment- and accretion-dominated metallicity evolution. We expect that while the normalization of the MZR declines with redshift, the slope of the correlation between metallicity and gas-mass at fixed stellar mass is not a strong function of redshift. Our results indicate that the gas fraction dependence of ‘regulator’ style models allows them to simultaneously explaining the shape, redshift evolution, and existence of correlated scatter with gas fraction about the MZR.

Key words: methods: numerical – galaxies: evolution – galaxies: general.

1 INTRODUCTION

Aging stellar populations within galaxies synthesize new heavy elements – or metals – which are redistributed within the interstellar medium (ISM). These metals enrich the ISM and are redistributed

via gas motion which imprints implicit information about each galaxy’s star formation history and baryon cycle. The distribution of metals within galaxies plays an important role in constraining our understanding of when galaxies acquire their fuel for star formation, where stars are formed, how the ejecta from the aging stellar populations is returned to the ISM, and the role that outflows may have in removing both mass and metals from the galaxy.

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Perhaps the most fundamental and early recognized relationship between galaxies and their metal content is the stellar-mass versus gas-phase metallicity relationship (hereafter, the mass–metallicity relationship, or MZR; Lequeux et al. 1979; Tremonti et al. 2004; Kewley & Ellison 2008). The MZR forms a tight correlation (i.e. scatter of ~ 0.1 dex) that has been observed over several orders of magnitude in stellar mass, over an order of magnitude in metallicity, and across a wide redshift range out to $z \sim 2$. The MZR shows that metallicity generally correlates with galaxy stellar mass such that low-mass galaxies tend to have lower metallicities than their higher mass counterparts. The MZR asymptotes around $M_* \approx 10^{10.5} M_\odot$ (e.g. Tremonti et al. 2004) yielding a nearly flat relationship between mass and metallicity for higher mass systems. The normalization of the MZR is observed to evolve slightly with time, with higher redshift galaxies having somewhat lower metallicities than their lower redshift counterparts (e.g. Savaglio et al. 2005; Erb et al. 2006; Maiolino et al. 2008; Lara-López et al. 2010; Zahid et al. 2014).

What remains missing is a clear physical understanding of why the metal content of galaxies tracks the stellar mass of galaxies as observed. Understanding the shape and evolution of the MZR alone has proven to be a challenging task. The first analytic, one-zone, simple chemical-evolution model that was developed to shed light on the driving forces behind the MZR and its evolution was the closed box model (Searle & Sargent 1972; Tinsley 1980). This model was made analytically tractable by assuming that (i) the total baryon content of the system is fixed (hence the ‘closed box’ title) and (ii) the evolution of the gas-mass, stellar mass, gas-phase metal-mass, and stellar-phase metal-mass is completely determined by star formation and the associated metal yield. Unfortunately, while the closed box model gives physical insight and yields clear predictions for the coevolution of galactic metals and galactic gas/stellar mass, it has now been widely established that the observed MZR cannot be directly explained with the fiducial closed box model alone (e.g. Chiappini, Matteucci & Gratton 1997; Tremonti et al. 2004). Numerous attempts have been made to extend and improve the closed box model’s ability to explain the MZR by accounting for inflows of pristine gas (e.g. going back to Larson 1972) or outflows of metal enriched gas (e.g. Larson 1974). Similar incarnations of the analytic gas and metal evolution equations first laid out in Larson (1972) and Larson (1974) continue to feature prominently in the literature as possible explanations for the shape, normalization, and evolution of the MZR (e.g. Dalcanton 2007; Finlator & Davé 2008; Peebles & Shankar 2011; Dayal, Ferrara & Dunlop 2013; Feldmann 2013; Lilly et al. 2013; Zahid et al. 2014).

Alternative modern interpretations of the MZR cast galaxies as more dynamic gas and metal reservoirs, subject to (and possibly dominated by) pristine gas inflows and enriched gas outflows (as in, e.g. Finlator & Davé 2008; Davé, Finlator & Oppenheimer 2012). In stark contrast to the closed box type models where galactic metallicity is a reflection of the integrated formation history of the galaxy, Finlator & Davé (2008) argued that the impact of inflows, outflows, and mixing implies that galactic metallicity is more likely set by the *current* galaxy properties. Specifically, the Finlator & Davé (2008) model defines an equilibrium metallicity as $Z_{\text{eq}} = \dot{M}_Z / \dot{M}_{\text{gas}}$ which is set by the *current rate* of new metal production and pristine gas inflow. Finlator & Davé (2008) and later Davé et al. (2012) showed that this reasonably simple and intuitive model is able to explain a number of features of the MZR including the slope of the low-mass end of the MZR, the turnover at higher masses, and the modified slope/normalization found in simulations with varied feedback scaling relations.

These analytic models act as broad tools that can be used to understand the average relationship between the gas-mass growth of a galaxy, production of stars and associated metal synthesis, metal retention, and ultimately galaxy metallicity evolution. However, these same models do not accommodate the varied formation tracks that real galaxies follow. As a result, the previously described simple analytic models do not shed light on the scatter in the MZR, and while these models do seem to describe the shape and normalization evolution of the MZR, they do not necessarily give insight into the actual evolutionary tracks along which individual galaxies evolve.

Addressing the scatter in the MZR is important because it has been argued that a galaxy’s position with respect to the MZR correlate with secondary galactic parameters, including the star formation rate (SFR; Ellison et al. 2008a). The correlations between the scatter in the MZR and SFR have been cast as a fundamental metallicity relationship that exists not just between metallicity and stellar mass, but also with SFR (e.g. Lara-López et al. 2010; Mannucci et al. 2010) or gas-mass (Bothwell et al. 2013). The existence of this correlated scatter about the MZR likely indicates a non-separable link between stellar mass, metallicity, and gas-mass. However, the slope of the correlation between gas-mass or SFR and offset from the MZR at a given stellar mass is not constant, and has been shown to depend on galaxy mass (Bothwell et al. 2013).

A different class of models have attempted to address the existence of correlated scatter about the MZR by allowing for deviations from the MZR (e.g. Lilly et al. 2013; Forbes et al. 2014). The key feature of these ‘regulator’ models is that the gas-mass in a system is allowed to vary, meaning that the metallicity of a system is dependent either explicitly on the current gas-mass (Lilly et al. 2013) or implicitly dependent on the current gas-mass via the recent accretion history of the system (Forbes et al. 2014). These ‘regulator’ models make concrete predictions for the existence of the correlated scatter about the MZR. Specifically, the Forbes et al. (2014) model predicts a correlation between galactic metallicity and SFR at a fixed stellar mass, where the slope of the correlation depends on the relative time-scale over which the accretion rates remain coherent against the time-scale over which a galaxy loses mass. The Forbes et al. (2014) model therefore predicts weaker correlated scatter about the MZR for higher mass systems, as is observed (e.g. Bothwell et al. 2013).

Despite their ability to match the observed nature of the correlated scatter in the MZR, the physical underpinnings of ‘regulator’ models have not been extensively tested via simulations. Numerical simulations can be leveraged to not only examine the emergence of the MZR (e.g. Davé et al. 2012, 2017; Torrey et al. 2014; Ma et al. 2016; De Rossi et al. 2017), but also inspect how individual galaxies evolve and to discriminate between the varied simple analytic models. Even with dozens of numerical simulation papers focused on the origin of the MZR and the correlated scatter about the MZR, comparatively little attention has been paid to individual galaxy evolution and scrutinizing the extent to which regulator models capture the physical processes that drive galaxies in their stellar mass, gas-mass, and metallicity evolution. Addressing this point seems particularly important, given that, e.g. even the best-fitting Forbes et al. (2014) regulator model requires scatter in accretion rates that is smaller than what is expected from N -body simulations.

In this paper, we explore the nature of the MZR as formed in the IllustrisTNG simulations. We use the large simulated galaxy population to compare the MZR against observations and quantify the existence of correlated scatter. Using the high-time–frequency snapshot output of the sub-boxes within the full IllustrisTNG volume, we then consider the detailed time evolution of galaxies to

identify the physical processes that drive the gas-mass, stellar mass, and metallicity evolution of the simulated galaxies. We compare our results with analytic MZR models in an attempt to validate the existing equilibrium and regulator model frameworks to better describe the MZR evolution seen in IllustrisTNG.

The structure of this paper is as follows: In Section 2 we describe the numerical simulations used in this paper (the IllustrisTNG simulation) with a focus on the metal enrichment and evolution methods. In Section 3 we present a global overview of the metal distribution within the IllustrisTNG simulation, including a breakdown of the metal retention efficiencies in various phases. In Section 4 we present the MZR across the redshift range $0 \leq z \leq 6$ along with a detailed description of the relationship between metallicity and galactic gas-mass. In Section 5 we consider the time evolution of individual galaxies to quantify the duration of galaxy deviations from the MZR and to address the physical processes that drive galaxies off the MZR. In Section 6 we give a discussion focused on the implications of our results for interpreting observations and understanding how our results compare with previous models. In Section 7 we summarize and conclude.

2 METHODS

The analysis presented in this paper is based on the IllustrisTNG simulation suite (Marinacci et al. 2017b; Naiman et al. 2018; Nelson et al. 2018a; Pillepich et al. 2018a; Springel et al. 2018). The IllustrisTNG project is an extension of the Illustris simulation project (Genel et al. 2014; Vogelsberger et al. 2014a,b; Sijacki et al. 2015), which includes a number of targeted improvements to the included galaxy formation model. The physical model employed in IllustrisTNG simulations builds on the original Illustris model (Vogelsberger et al. 2013; Torrey et al. 2014) with important updates and modifications described in Weinberger et al. (2017) and Pillepich et al. (2018b). The IllustrisTNG simulation suite consists of three simulation volumes: TNG50, TNG100, and TNG300. The IllustrisTNG simulations have been used to study the size evolution of galaxies (Genel et al. 2018), the enrichment of the intercluster medium (Vogelsberger et al. 2018), and the impact of AGN feedback on galaxy quenching (Weinberger et al. 2018). For the analysis presented in this paper, we use the TNG100 simulation which is an analogue to the Illustris-1 simulation, with the updated physical model and cosmology consistent with the 2015 Planck collaboration results (Planck Collaboration XIII 2016). We refer interested readers to the introductory papers for further details beyond the brief description provided here.

2.1 Metal enrichment

Here we briefly summarize the metal enrichment procedures that are employed in the IllustrisTNG model. Stars are formed from dense gas ($n_{\text{H}} \gtrsim 0.13 \text{ cm}^{-3}$) using a star formation prescription that is designed to reproduce the Kennicutt–Schmidt relation (Springel & Hernquist 2003). Simulation star particles record their birth time and are assigned the same metallicity as the ISM gas from which they were born. Simulation star particles in the high-resolution TNG100 simulation (which we study exclusively in this paper) have masses of $m_* \sim 10^6 M_{\odot}$ and therefore represent an unresolved large population of real stars. Each unresolved stellar population is assumed to be comprised of a Chabrier (2003) initial mass function (IMF).

As star particles age, mass and metals from the aging stellar populations are returned to the ISM. At any time-step, stellar

lifetime tables (Portinari, Chiosi & Bressan 1998) are used to determine which stars within the unresolved full stellar population are expected to be moving off the main sequence. Mass return and metal yield tables for SNIa (Nomoto et al. 1997), SNI (Portinari et al. 1998; Kobayashi et al. 2006), and AGB stars (Karakas 2010; Doherty et al. 2014; Fishlock et al. 2014) are then used to determine the amount of mass and metals that should be returned to the ISM. The mass and metal return is carried out by finding 64 nearest gas cells and spreading the returned gas-mass and metal-mass among them. This mass and metal return procedure leads to a time- and spatially dependent enrichment of the ISM based on the distribution and formation history of the stellar population in any galaxy. After metals are deposited in the ISM, they are passively advected with the fluid flow.

Galactic winds are probabilistically driven in the IllustrisTNG model based on the local SFR (for full details, see Pillepich et al. 2018b). Specifically, all cells are assigned a mass outflow launching rate of $\dot{M}_{\text{wind}} = \eta_{\text{wind}} \dot{M}_{\text{SFR}}$, where η_{wind} is the wind mass loading factor and \dot{M}_{SFR} is the local SFR. The IllustrisTNG prescription for the wind mass loading factor is given by

$$\eta_{\text{wind}} = \frac{2}{v_{\text{wind}}^2} e_{\text{wind}} (1 - \tau_{\text{wind}}), \quad (1)$$

where v_{wind} is the wind outflow velocity, e_{wind} is the available energy to launch winds, and τ_{wind} is the fraction of available energy assumed to go into heating the gas (i.e. the thermal fraction). A full and detailed description of how each of these terms is set, and how this differs from the previous Illustris model, can be found in section 2.3.2 of Pillepich et al. (2018b). However, for this paper, we note that the adopted wind launching parameters result in an approximate scaling of the wind mass loading of $\eta_{\text{wind}} \propto M_{200c}^{-5/6}$ (see Pillepich et al. 2018b, section 3.2.1). We note that the adopted prescriptions for outflows directly impact the baryon cycle in-and-around galaxies, and therefore many of the results presented in this paper.

Additionally, the winds are assigned a metallicity which is lower than the ambient ISM (specifically, $Z_{\text{wind}} = 0.4Z_{\text{ISM}}$). Metal-mass not launched in the wind is left in the ISM, such that metal-mass is conserved. The reduction in wind metallicity is motivated by the fact that winds are expected to entrain a significant amount of material as they propagate away from their launch site. Entrainment of low or lower metallicity gas – as is likely to be the case for off-disc-plane material – will naturally dilute the wind metallicity. Since the IllustrisTNG SF driven winds are hydrodynamically decoupled for a brief period, we adopt a lowered metallicity to account, in part, for any low-metallicity gas entrainment which may have occurred. The reduction in wind metallicity was tuned to encourage a better match to the MZR in the Illustris model (Vogelsberger et al. 2013; Torrey et al. 2014) and remains unchanged in the IllustrisTNG set-up.

2.2 Definition of metallicity and ISM mass

In this paper we focus our attention on the evolution of galactic gas-phase metallicity, with a further emphasis on comparisons with observations of extragalactic nebular emission line based metallicity measurements. To make simple comparisons with nebular emission line metallicity measurements, gas-phase metallicity values quoted in this paper are SFR weighted metallicity values. Using SFR weighted metallicity measurements limits the sample of galaxies that have assigned metallicities to those with star-forming gas. Throughout this paper, we therefore require non-zero SFRs in order to quote metallicity values. In some portions of the paper (where

explicitly noted) we require higher star formation threshold values be met in order to further remove nearly quenched galaxies that would likely not be observationally detectable.

We quote two distinct metal abundance values in this paper. When discussing ‘metallicity’, we adopt the scalar metallicity value from the simulation, $Z = M_{Z,\text{gas}}/M_{\text{gas}}$, which we define in the traditional way as the fraction of gas-mass that is composed of metals.

When making comparisons with nebular emission line determined metallicities [quoted as $\log(\text{O}/\text{H}) + 12$ values] we also use the global metallicity scalar, assuming that oxygen is 35 per cent of the metal-mass. In addition, we use SFR-weighted metallicities for each galaxy, in order to provide a more even handed comparison with nebular emission line measurements. We do not place any emphasis on the absolute normalization of the simulated or observed MZR values since it is well established that nebular emission line metallicity diagnostics have factor of >2 uncertainty in their absolute normalization (Kewley & Ellison 2008). Instead we focus our attention on the shape and normalization evolution of the MZR.

Additionally, in several places in this paper we discuss the co-evolution of galactic metallicity and ISM mass. We adopt an ISM mass definition as being the total mass of gas over which the metallicity was calculated. Since in this paper we use SFR-weighted metallicities, our adopted ISM mass definition is therefore the total mass of gas above our employed star formation density threshold of $n_{\text{H}} \gtrsim 0.13 \text{ cm}^{-3}$.

3 RESULTS: GLOBAL METAL DISTRIBUTION

In this section we explore the broad characteristics of the gas-mass and gas-phase metal-mass distribution in the TNG100 simulation. We first consider global density–temperature phase diagrams of both the gas- and metal-mass distribution, and then consider the contributions to these global phase diagrams from galaxies of varied masses. Finally, we show the evolution of the metal retention efficiencies for the ISM, circumgalactic medium (CGM), and stars.

3.1 Global gas-mass and metal-mass density–temperature phase diagrams

Fig. 1 shows a density–temperature phase diagram of the global distribution of gas-mass (left) and gas-phase metal-mass (right). Thin black lines have been placed to mark boundaries between four loosely defined regions within this phase diagram: hot gas ($T > 10^7 \text{ K}$), warm-hot gas ($10^5 \text{ K} < T < 10^7 \text{ K}$), diffuse material ($\rho < 1000\rho_c\Omega_b$; $T < 10^5 \text{ K}$), and condensed material ($\rho > 1000\rho_c\Omega_b$; $T < 10^5 \text{ K}$). These are the same phase boundaries originally employed in Davé et al. (2001) which were also used more recently to analyse the original Illustris simulation in Haider et al. (2016). The fraction of gas-mass (left) or metal-mass (right) in each region is indicated within the figure.

Generally, the phase-diagram mass distribution for IllustrisTNG is qualitatively identical to what was found in the original Illustris simulation (e.g. Haider et al. 2016). The ISM mass is described by a characteristically thin distribution that is set by the Springel & Hernquist (2003) equation of state model used in the IllustrisTNG simulations which. The ISM mass can be easily identified as a thin feature in the dense portion of the phase diagram. The majority of the redshift $z = 0$ IllustrisTNG gas (49.5 per cent) is in the WHIM intermediate temperature range, which is a similar fraction to what was found in the original Illustris (57.8 per cent). The hot phase gas contains 7.5 per cent of the $z = 0$ IllustrisTNG gas, which is a marginal increase from the original Illustris (7.0 per cent). There

are, however, some more notable changes in the content of the diffuse and condensed regions. While the diffuse gas increased from 23.2 per cent in Illustris to 38.9 per cent in IllustrisTNG, the condensed gas decreased from 12.0 per cent in Illustris to 4.2 per cent in IllustrisTNG. The modification to the condensed gas fraction is likely a result of the modified stellar and AGN feedback used in IllustrisTNG compared against Illustris.

Additionally, the uncorrected equation of state for the low-density/temperature IGM material showed some curvature in IllustrisTNG, which was not present in Illustris and which is not consistent with expectations for the power-law density–temperature relation governing gas in this regime. This curvature in the IGM equation of state was the result of minor, but incorrect, numerical heating associated with expansion of gas in very low density environments. While this effect does not impact any of the results presented in this paper in any substantive way, we nevertheless apply an appropriate temperature correction to the plotted phase diagrams such the low-density gas (i.e. $\rho < 10^{-6} \text{ cm}^{-3}$) follows the appropriate power law relation. Specifically, the adiabatic IGM material is identified by finding the maximum density of material in the phase diagram for gas in the regime $\rho < 10^{-6} \text{ cm}^{-3}$ and $T < 10^{4.5} \text{ K}$. All material in that density range then has a temperature correction applied such that the corrected adiabatic equation of state material follows the expected $T \propto \rho^{\gamma-1}$ (see Martizzi et al. 2018 for further details).

In this section and throughout this paper, our primary focus is on comparing the gas-mass distribution against the metal-mass distribution as a tool for understanding the metallicity evolution of IllustrisTNG galaxies. The distribution of gas-mass within the density–temperature phase diagram shown in the left-hand panel of Fig. 1 can be contrasted against the gas-phase metal-mass distribution shown in the right-hand panel of the same figure. As with the gas-mass, the majority of the gas-phase metals are in the WHIM (64.2 per cent), with 15.4 per cent being found in the condensed region and 14.9 per cent being found in hot gas. In stark contrast with the gas-mass distribution, a very small fraction (5.5 per cent) of metals are found in diffuse gas. This is consistent with a basic picture of galaxy formation and metal production where metals are produced deep within galactic potentials and mostly pollute the gas in and immediately around the galaxies where they form. However, importantly, it is worth noting that while all star formation is associated with gas in the ‘condensed’ region of phase space, the majority of gas-phase metals (~ 85 per cent) are found outside of this region. Feedback from stellar winds and AGN are critical components of the baryon cycle in our simulations, with the resulting metal distribution being spread over a wide range of the density-temperature phase diagram. From Fig. 1 we can conclude that the majority of metals live outside of the ISM in the IllustrisTNG model at redshift $z = 0$. Although not shown in Fig. 1, we have further confirmed that the majority of gas-phase metals reside outside of the ISM over the redshift range $0 < z < 3$. At higher redshifts ($z > 3$) a fraction greater than 50 per cent of metals reside in the condensed region of phase space.

3.2 Distribution of metals around galaxies

To further investigate the distribution of mass and metals around IllustrisTNG galaxies, Fig. 2 shows density–temperature phase diagrams for the gas-mass (top row) and gas-phase metal-mass (bottom row) for gas that is bound to galaxies with average masses of $M_* = 10^9 M_\odot$ (left column), $M_* = 10^{10} M_\odot$ (centre column), and $M_* = 10^{11} M_\odot$ (right column). The phase diagrams

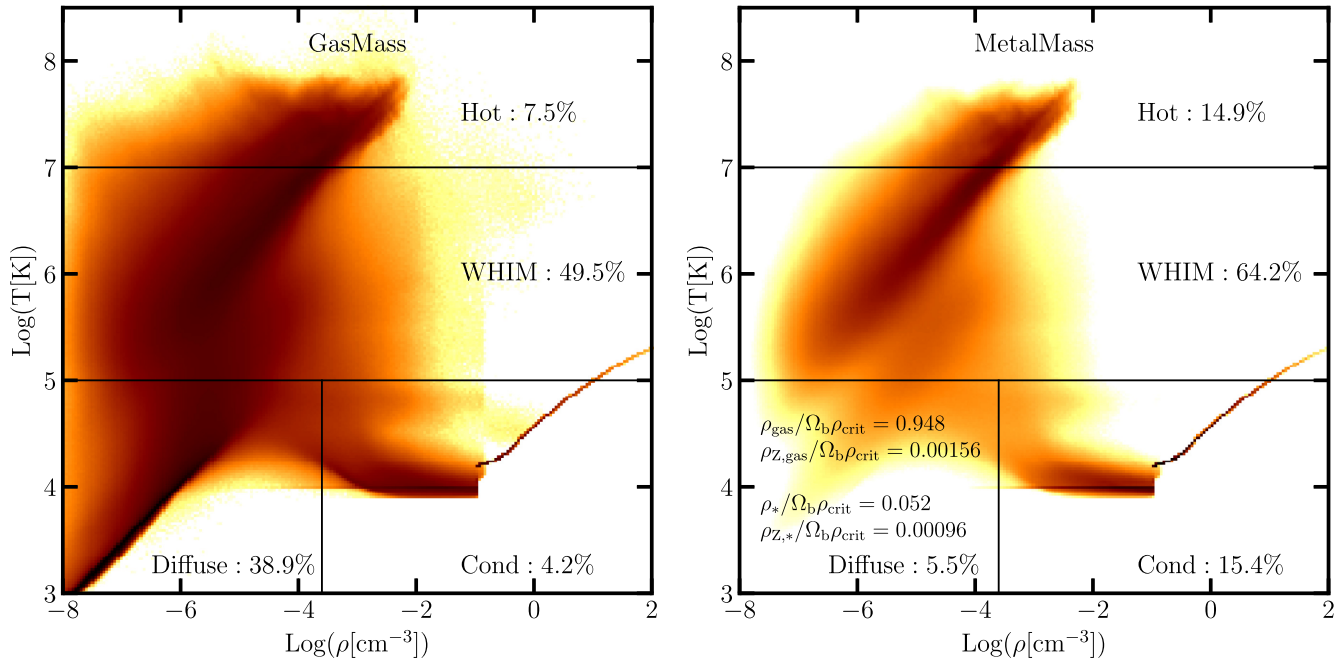


Figure 1. Phase diagrams showing the redshift $z = 0$ global distribution of gas-mass (left) and gas-phase metal-mass (right) as a function of density and temperature. Thin black lines indicate boundaries used to separate the hot, warm-hot intergalactic medium (WHIM), diffuse, and condensed material (Davé et al. 2001; Haider et al. 2016). The fractions of gas-mass (or gas-phase metal-mass) within each region is indicated within the plot. There is a significantly higher relative fraction of metals in the condensed region of phase space, which is where star formation occurs and metals are produced. However, there is also significant pollution of the WHIM and hot regions of phase space, with ~ 85 per cent of gas-phase metals being outside of the condensed region. A correction to the temperature of the low-density IGM has been applied as discussed in the text.

were constructed by taking all gravitationally bound gas in the SUBFIND catalogue (Springel, White & Hernquist 2001; Dolag et al. 2009) for the 100 galaxies most closely matched in mass to the three respective target masses. Within each figure, dashed lines indicate boundaries that are used to separate the hot CGM (top region), cool-diffuse gas (lower left), and dense ISM (lower right). We define here the hot CGM as being gas above the line $\log(T/10^6 \text{ K}) = 0.25 \log(n/405 \text{ cm}^{-3})$, which is the same boundary employed in Torrey et al. (2012b). The hot CGM gas boundary used here cuts orthogonally through the gas-mass distribution within the phase diagram at a location of low gas density, which makes our quoted mass results reasonably insensitive to the exact normalization adopted. As outlined in Section 2, we define the ISM gas as being material above our employed star formation density threshold of $n_{\text{H}} \gtrsim 0.13 \text{ cm}^{-3}$. The amount of material (gas-mass, or metal-mass) within each region is printed in the figure, as is the average metallicity of gas in each region.

Examining first the gas-mass distribution within these phase diagrams, we find that there is a significant and well-defined population of gas in each of the regions at all of the galaxy mass scales. As in the global phase diagram, the ISM mass can be easily identified based on the thin Springel & Hernquist (2003) equation of state model. At redshift $z = 0$ (where the phase diagrams were constructed) the ISM is spatially confined to a region in the centre of each halo: namely a central star-forming gas disc extending between one and a few kiloparsecs in length. The cool-diffuse gas acts as a continuation of the dense ISM gas, extending down 2–2.5 orders of magnitude in density. While a fraction of it is associated with the cool-diffuse gas is an extended gas disc, some of the material is distributed further out into the CGM and can be considered a cool CGM component. The hot CGM gas is clearly distinct from the

other two populations of gas, is generally hotter for more massive galaxies, and spatially occupies the entire halo.

The gas-phase metal-mass distribution broadly traces the gas-mass distribution, but is biased towards the cool-diffuse gas and ISM. This is seen quantitatively by the higher metallicities obtained for the ISM compared against the CGM gas. The distinction between ISM and CGM metal content and metallicity is most pronounced for the two lower mass systems where the ISM metallicity is ~ 5 –6 times higher ($Z_{\text{CGM}} = 0.1 Z_{\odot}$; $Z_{\text{ISM}} = 0.6 Z_{\odot}$ for the lowest mass bin). The higher mass galaxies still have enhanced ISM metallicities, but with a somewhat smaller offset (a factor of ~ 3 –4).

Importantly, we note that the IllustrisTNG simulated galaxies host a significant fraction of their gas-mass and gas-phase metal-mass outside of the ISM in either the cool-diffuse gas, or in the hot CGM. This point is important when considering the applicability of, e.g. closed or leaky box models in describing the metallicity evolution of galaxies. Tracking the metallicity evolution of the ISM requires accounting for both the production of new metals associated with star formation as well as the constant shifting of those metals between different phases. The enrichment of ISM, cool-diffuse gas, or the CGM relies on a competition between pristine gas inflow naturally associated with cosmological galaxy growth and the injection of new metals either directly associated with star formation or associated with enriched gas accretion/outflows. For the galaxies considered here, there is a trend where the highest metallicity gas resides in the ISM at the centre of the halo. However, the metal budget in the cool-diffuse gas and CGM is generally larger than the ISM metal-mass budget itself (Peebles et al. 2014).

To further explore galaxy metal retention and the relative distribution of metals amongst the gas phases, we define a quantity that

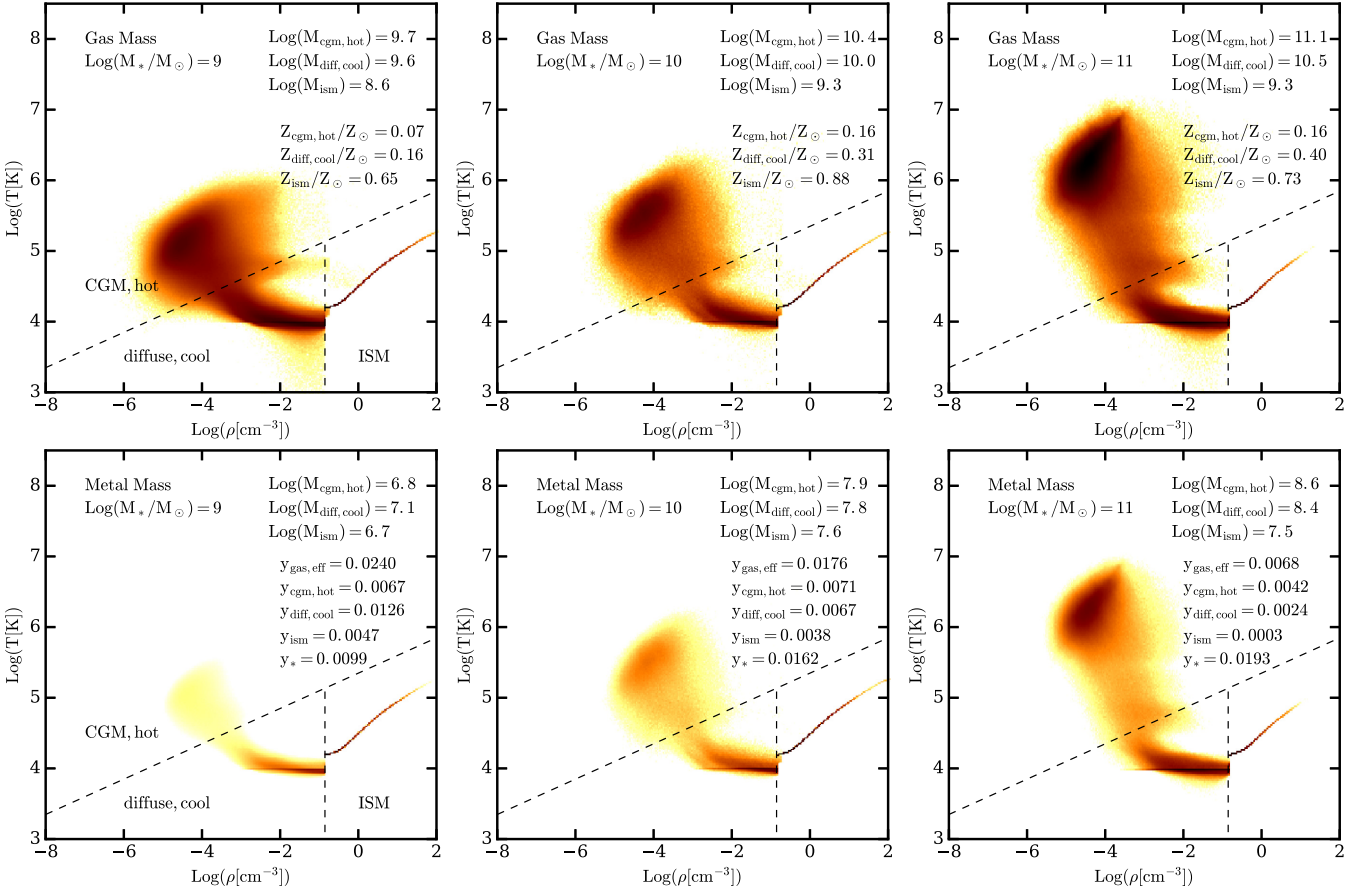


Figure 2. Density–temperature phase diagrams indicating the distribution of gas-mass (top row) and gas-phase metal-mass (bottom row) for galaxies with stellar masses of $M_* \approx 10^9 M_\odot$ (left column), $M_* \approx 10^{10} M_\odot$ (centre column), and $M_* \approx 10^{11} M_\odot$ (right column). We split the gas distribution into three regions indicated by thin dashed lines: the hot CGM material (top region), the dense/cool ISM gas (bottom right), and the diffuse/cool gas (bottom left). The total gas-mass – or gas-phase metal-mass – in each region is indicated within each figure. The average metallicity of gas in each region, or the retained metal yield for each region ($y_i = M_{Z,i}/M_*$; see main text for further details) is indicated within the plot.

we refer to as the retained metal yields which are printed within the bottom row of Fig. 2. The metal yield, y , is used to calculate the total amount of metal-mass produced from stars according to $M_Z = yM_*$. Our defined retained metal yields are motivated by the metal yield, but are calculated independently for several gas phases as well as the stellar component. In every case, the retained metal yield γ is defined as

$$\gamma_i = \frac{M_{Z,i}}{M_*}, \quad (2)$$

where $M_{Z,i}$ is the total metal-mass in that phase and M_* is the total stellar mass of the galaxy.¹ The quoted retained metal yields are averages across all galaxies falling into each mass bin. These retained metal yields are useful because they indicate the combined influence of metal enrichment and metal retention efficiency of each phase, and we refer to these factors interchangeably as retained metal yields and metal retention efficiencies in the subsequent text. The total retained metal yield γ_{tot} gives a combined measure of the metal retention within all gas in the galaxy, with the phase-separated metal yields indicating how those metals are partitioned between the

¹We note that while we discuss the metal yield for stars to retain consistency with the gas phases, the ‘stellar metal yield’ as defined here is simply the stellar metallicity $y_* = M_{Z,*}/M_* = Z_*$.

Table 1. Retained metal yields at $z = 0$ for the defined gas phases in three mass bins.

M_*	$10^9 M_\odot$	$10^{10} M_\odot$	$10^{11} M_\odot$
$\gamma_{\text{all baryons in halo}}$	0.0348	0.0338	0.0271
$\gamma_{\text{all gas in halo}}$	0.0240	0.0176	0.0068
γ_{ISM}	0.0047	0.0038	0.0003
$\gamma_{\text{cool,diff}}$	0.0126	0.0067	0.0024
$\gamma_{\text{hot,CGM}}$	0.0067	0.0071	0.0042
γ_{stars}	0.0099	0.0162	0.0193

various gas phases or stars within the galaxy. Table 1 summarizes the average retained metal yields calculated for three mass bins at redshift $z = 0$.

For the IllustrisTNG galaxies, the total gas retained metal yield *decreases* with increasing stellar mass from $\gamma_{\text{eff}} = 0.024$ for the lowest galaxy mass bin considered to $\gamma_{\text{eff}} = 0.007$ for the highest galaxy mass bin. The decreasing retained metal yield is an indication that the more massive galaxies are more efficient at removing metal-mass from any/all of the gas phases when compared against their lower mass counterparts. Gas-phase metal removal can be achieved by either (i) locking an increasingly large fraction of metals into stars, or (ii) by ejecting metals from the halo entirely. To distinguish

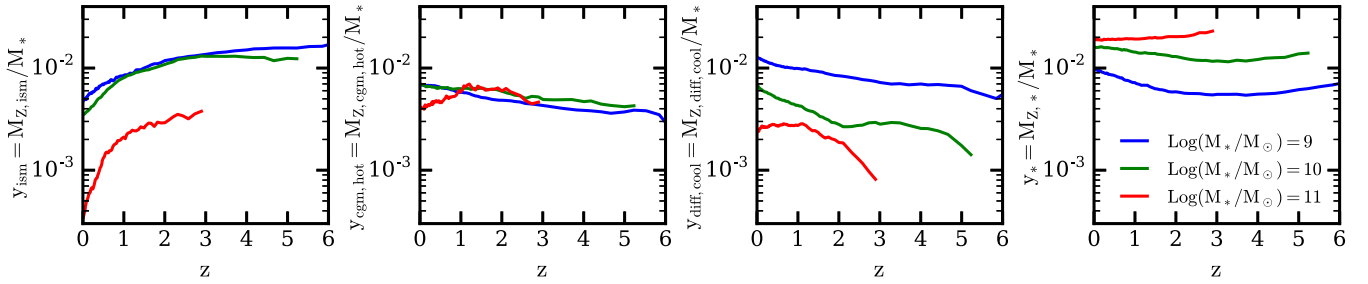


Figure 3. The retained metal yield ($y_i = M_{Z,i}/M_*$; see text for further details) for the ISM (left), the hot CGM (centre-left), the diffuse cool gas (centre-right), and stars (right) as a function of redshift. The retained metal yields are a normalized parameter indicating the galactic metal retention within each phase. The retained metal yield shown here has been calculated for three mass bins in each panel based on the 100 galaxies with masses closest to the target mass. Lines are omitted when the bin size becomes larger than 0.1 dex. Although metals are produced from star formation in dense ISM gas, the retained metal yield for the ISM is low. There is a clear trend where galaxies decrease (increase) the amount of metals they store in the diffuse-cool gas (stars) as their stellar mass increases. The largest reservoir of metals for low-mass galaxies is the diffuse cool gas, whereas the largest reservoir of metals for high-mass galaxies is locked into stars.

between these two possibilities, we need to know the total metal yield for the IllustrisTNG simulations.

The global yield for metals in the IllustrisTNG simulations is set by the adopted IMF along with the adopted metal yield tables (both discussed in Section 2), and is influenced by the age distribution and metallicity distribution of stellar populations in the simulation. The global metal yield cannot be directly analytically calculated owing to the dependence on the age and metallicity distribution of stellar populations (Nelson et al. 2018a), but can be calculated from the global stellar mass density and metal-mass density

$$y_{\text{global}} = \rho_Z / \rho_* \approx 0.05. \quad (3)$$

This global metal yield has been derived for redshift $z = 0$ and will increase somewhat with decreasing redshift owing to the evolving age and metallicity distribution of the stellar populations. The retained metal yield of $y_{\text{eff}} = 0.024$ for all gas in the low-mass galaxies only accounts for half of the total metal yield.² The remaining half of the metals produced by these low-mass galaxies are split between being locked into stars (about 20 per cent) and being ejected from the galaxy (about 30 per cent). In the highest mass bin, the retained metal yield for all gas drops significantly to $y_{\text{eff}} = 0.007$ (roughly ~ 15 per cent), but the amount of metals locked into stars significantly increases (roughly ~ 40 per cent), meaning that just under half of the metals produced have been ejected from the galaxy. High-mass IllustrisTNG galaxies ($\gtrsim 10^{11} M_\odot$) are less efficient at retaining their metals when compared against their lower mass companions. The relatively high efficiency of metal ejection for high-mass galaxies can likely be attributed to AGN feedback in our model as has been found to be the case in previous studies (e.g. Suresh et al. 2015). However, we note that the specific role of any feedback processes (e.g. AGN/stellar feedback) or physical processes (e.g. ram-pressure or tidal stripping) are not individually investigated in this paper. The broad picture painted in Fig. 2 is that redistributing metals between different gas phases is important in determining the ISM metallicity.

²We note that not every galaxy will have an identical metal yield given their unique metallicity and formation histories. All quoted retention efficiencies should therefore be treated as approximate.

3.3 Time evolution of metal retention efficiencies

Fig. 3 shows the time evolution of the retained metal yield for the ISM (left), the hot CGM (centre left), the cool-diffuse gas (centre right), and stars (right). As in Fig. 2, the retained metal yields shown in Fig. 3 indicate the total retained metal yield from the 100 galaxies with masses closest to the target value. Lines are omitted where the 100 closest galaxies span more than 0.1 dex in stellar mass. We emphasize that these lines shown are for independent galaxy selections at each redshift, and are not tracking individual galaxies or galaxy populations in time.

In general, the retained metal yield for the stars and the hot CGM remains reasonably static with time. The hot CGM retains an retained metal yield of ~ 0.003 – 0.008 which represents roughly ~ 5 – 15 per cent of the metal budget for all of the three galaxy mass bins out to redshift $z = 3$. Stars retain a metal yield that depends clearly on the total stellar mass of the system, but remains reasonably static with time. The time-independence of the stellar metal yield is an indication that stellar mass is more important in determining stellar metallicity than redshift in the IllustrisTNG model, with higher mass galaxies having higher metallicity stars.

The cool-diffuse gas and ISM phases show more pronounced evolution with time. The ISM metal yield increases with increasing redshift similarly for all the three galaxy mass bins. The highest mass bin is offset towards lower values by a factor of ~ 8 , as was discussed in the previous subsection for redshift $z = 0$. The general trend of increasing ISM retained metal yield with increasing redshift indicates that higher redshift galaxies keep a higher fraction of their metals in their ISM compared against their low-redshift counterparts. We return to the discussion of these retained metal yields (or metal retention efficiencies) when addressing the evolution of the MZR.

4 RESULTS: METAL DISTRIBUTION AND EVOLUTION IN GALAXIES

4.1 Metal distribution within galaxies

Fig. 4 shows face-on projections of galaxies with stellar masses $M_* \approx 10^{10} M_\odot$ from the TNG100 simulation. The three rows show the gas surface density (left), the SFR surface density (centre), and the mass-weighted average metallicity (right). Associated colour bars for each panel are shown at the top of each column. The field of view is 50 kpc wide in each image. The specific systems shown

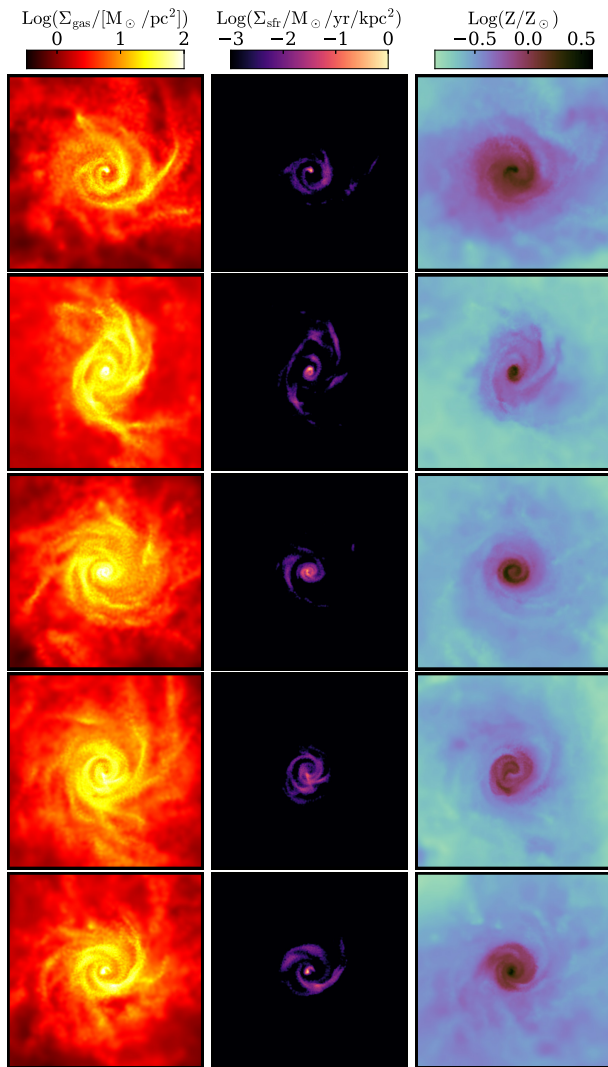


Figure 4. Projections of several gas properties for five galaxies with masses $M_* \approx 10^{10} M_\odot$ from the TNG100 simulation showing the gas surface density (left), the SFR surface density (centre), and the gas-phase mass-weighted average metallicity (right). Associated colour bars for each panel are shown at the top of each column. Face on projections were achieved by projecting the galaxy properties along the net angular momentum axis for gas above the star formation density threshold. Each image shows a field of view that is 50 kpc on a side.

are the five galaxies with masses closest to $M_* = 10^{10} M_\odot$ with SFRs greater than $1 M_\odot \text{ yr}^{-1}$. The SFR cut was employed to ensure star-forming galaxies with prominent gas discs. The projections are taken to be along the angular momentum vector for all star-forming gas in the galaxy, leading to roughly face on projections of the central gas disc.

The gas surface density distribution gives a sense for the structure and resolution of galaxies in IllustrisTNG. The five systems shown in this panel have total gas-masses of $M_{\text{gas}} \approx 10^{10.75} - 10^{11} M_\odot$, meaning they are resolved with roughly $N_{\text{gas}} \approx 3 - 5 \times 10^4$ gas elements. This number of gas cells allows for the resolution of a radial surface density profile, as well as some internal structure in the gas disc. The star formation surface density closely traces the high-density gas. The star-forming gas is confined to the central region of each galaxy, with enhanced star formation activity along the dense spiral arm gas features. Although we do not show it here,

young stars closely trace the star formation surface density, which serve as sites of rapid heavy element enrichment.

The gas metallicity shown in the third column was calculated as a mass-weighted average of the gas phase metallicity.³ The peak central metallicity for this galaxy sample is slightly above solar. We find there is a metallicity gradient present where the high central metallicities fall off rapidly and nearly monotonically with radial distance. For the selected galaxies shown, the magnitude of this total metallicity drop is of order ~ 0.5 dex over the central ~ 10 kpc. At larger radii (i.e. towards the edge of the frames) the low-metallicity gas outside of the central gas disc shows a less pronounced metallicity gradient. The metallicity gradient is influenced by two competing effects: localized enrichment from aging stellar populations and gas mixing between radial bins via gas inflows and outflows (e.g. Rich et al. 2012). The metallicity of the gas near the centrally concentrated star-forming regions is continually increased as stellar populations enrich the local ISM – which increases the metallicity gradient prominence. However, as can be inferred from the surface density plots in the left column, most of the discs have clear non-axisymmetric features, leading to a radial redistribution of metals – which decreases the metallicity gradient. The presence of a metallicity gradient is consistent with lower metallicity gas being found in the diffuse-cool gas and hot CGM of the phase diagrams presented in the previous section.

Fig. 5 shows the same quantities as Fig. 4, but now for galaxies with masses $M_* \approx 10^{11} M_\odot$. The more massive galaxies share a number of characteristics with their lower mass counterparts, including identifiable gas discs with dense spiral patterns which coincide with ongoing star formation. However, whereas all five of the lower mass galaxies featured a well-ordered and monotonically decreasing gas surface density profile, the five more massive galaxies show visible distortions, and in some cases significantly depressed central gas densities. The gas distortions and depressed central gas densities are the result of AGN feedback, which is more impactful to massive galaxies in the IllustrisTNG model. The presence of strong feedback has a ripple effect on the metallicity measurements, with metallicity gradients being less pronounced. The same strong feedback which can be seen to influence the gas distributions in Fig. 5 is responsible for the diminished mass content and ‘metal yield’ for the ISM and cool-diffuse medium discussed in the previous section.

For all subsequent portions of this paper, we will quote galaxy metallicities as a single quantity per galaxy. We specifically calculate galaxy metallicities as being an SFR weighted average metallicity since the majority of observations of gas-phase metallicity rely on nebular emission lines, which probe gas associated with star-forming regions. Comparing the second and third columns, it can be seen that the SFR weighted metallicities will be biased towards the central, dense gas within our galaxy populations.

4.2 The illustrisTNG MZR

Fig. 6 shows the gas-phase mass–metallicity relation at six distinct redshifts. The black-and-white coloured two-dimensional histograms indicate the distribution of simulated galaxies within this space, with the solid black lines and shaded bands indicating in median and 1σ scatter of the simulated galaxy distribution. Where

³We use mass weighted, rather than SFR weighted, gas phase metallicity here to provide a continuous map, rather than simply highlighting the star-forming gas.

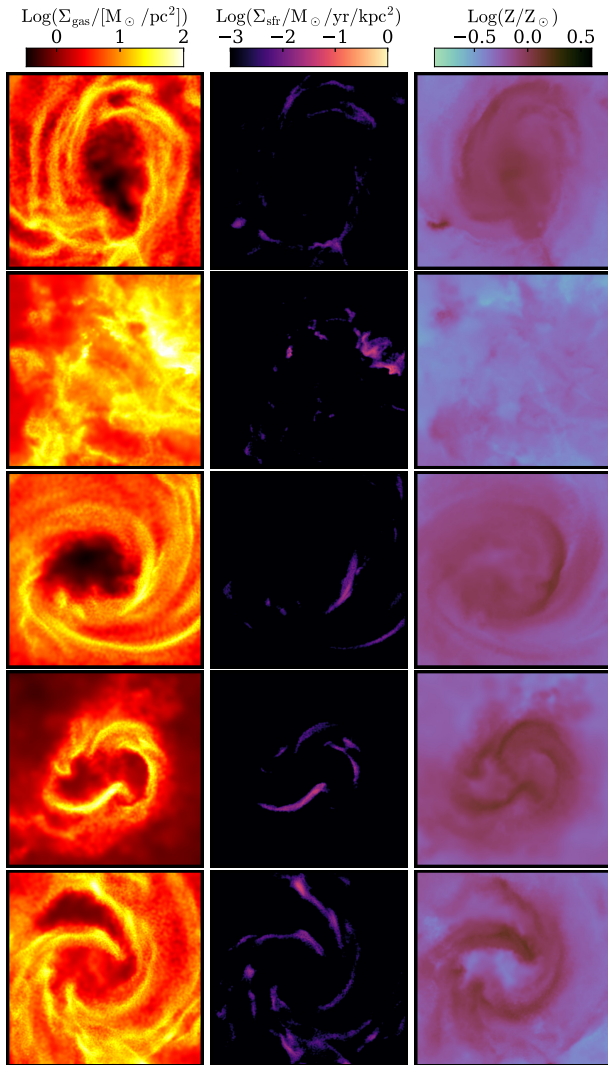


Figure 5. Same as Fig. 4, except for galaxies selected around $M_* \approx 10^{11} M_\odot$. The higher mass galaxies considered here have less well-ordered gas discs owing to the increased prominence of AGN feedback, and have less clearly identified metallicity gradients.

available, we have included median data points for the MZR from the observational literature including Tremonti et al. (2004), Zahid et al. (2011), and Erb et al. (2006). At redshift $z = 0$, the simulated MZR shows a clear trend of increasing metallicity with increasing stellar mass, up to roughly $M_* \approx 10^{10-10.5} M_\odot$. The slope of the $z = 0$ simulated MZR is broadly consistent with the observational data, but may be marginally shallower than the observed slope. This is interesting given the strong/steep scaling of the outflow mass loading factor with galaxy mass adopted in the IllustrisTNG model. It is possible that either by increasing the steepness of the outflow mass loading factor scaling with galaxy mass (which could cause tension with the galaxy stellar mass function constraints), or by allowing for a non-constant metal loading factor (e.g. as discussed in Peebles & Shankar 2011), that better agreement could be obtained between the simulated and observed MZR slopes.

We see a flattening in the MZR beyond $M_* \approx 10^{10-10.5} M_\odot$, which is frequently referred to as the saturation metallicity. The mass range $M_* \gtrsim 10^{10.7} M_\odot$ is sparsely populated because we only consider galaxies with active/ongoing star formation (i.e. $SFR > 0$).

The overall shape of the $z = 0$ MZR compares favourably with observations, with the exception that the simulated MZR appears to begin flattening at somewhat lower masses when compared against the observations. This metallicity underestimate at the high-mass end may be in part due to contamination with nearly quenched galaxies, as we will discuss later in this Section.

In contrast to the $z = 0$ MZR, the high-redshift MZRs also contain a break in the low-mass MZR slope at $M_* \approx 10^9 M_\odot$. No similar break in the low-mass MZR slope was present in the original Illustris model (e.g. Torrey et al. 2014). These bumps are the product of the minimum wind velocity imposed in IllustrisTNG stellar feedback model. Wind velocities are assigned within the IllustrisTNG model according to

$$v_w = \max \left[\kappa_w \sigma_{\text{DM}} \left(\frac{H_0}{H(z)} \right)^{1/3}, v_{w,\text{min}} \right], \quad (4)$$

where $\kappa_w = 7.4$ is the wind velocity normalization factor, σ_{DM} is the local dark matter velocity dispersion, and $v_{w,\text{min}} = 350 \text{ km s}^{-1}$ is the minimum allowed wind velocity (see Pillepich et al. 2018b; eq. 1 and table 1). Low-mass galaxies in the IllustrisTNG model will have low dark matter velocity dispersions, and will therefore be assigned the minimum wind velocity. The transition scale for the fiducial to constant wind velocity is not directly set by stellar mass, but roughly corresponds to $M_* \sim 10^9 M_\odot$ which is where the MZR bumps are visible. At the fixed wind velocity of $v_{w,\text{min}} = 350 \text{ km s}^{-1}$, the amount of gas ejected in winds (i.e. the wind mass loading factor) is lower than what would have been ejected if the wind velocity were permitted to be lower. The reduced ejected wind mass and larger-than-expected wind velocity results in longer wind recycling times and less direct metal ejection, which manifests as somewhat higher metallicities for low-mass galaxies. MZR data for lower galaxy mass bins are more scarce, but there is not currently strong observational evidence in agreement, or disagreement, with the break in the MZR found in our models. While the constant minimum wind velocity is critical in the IllustrisTNG model towards matching the low end of the galaxy stellar mass function (Pillepich et al. 2018b), it also leaves a clear potentially observable imprint on the MZR. Further observational data on the low-mass MZR may help constrain the validity of the adopted minimum wind velocity assumption.

4.3 Redshift evolution of the illustristng MZR

In general, the median MZR from the simulations and observations compare favourably where data exist out to $z = 2$ (see Fig. 6). While we place limited emphasis on the absolute normalization of the MZR (Kewley & Ellison 2008), there is a normalization evolution between redshifts $z = 0$ and $z = 2$ that is present in the observed data and which appears to be captured in the simulations. Our simulations make clear predictions for the continued evolution of the MZR out to high redshift which will likely be testable in the near future with JWST. The O III, N II, H α nebular emission lines will shift into JWST NIRSPEC instrument for $z \gtrsim 4$, which will likely lead to a large influx of metallicity data for these high-redshift galaxy populations. Our models predict that the gradual decrease in MZR normalization that has currently been observed out to redshift $z \sim 2$ will continue out to higher redshift yet.

Fig. 7 provides some guidance on the magnitude of this expected continued evolution. The solid curves in Fig. 7 show the metallicity evolution as a function of redshift for several mass values. The dashed lines show the best-fitting lines determined via a chi-squared

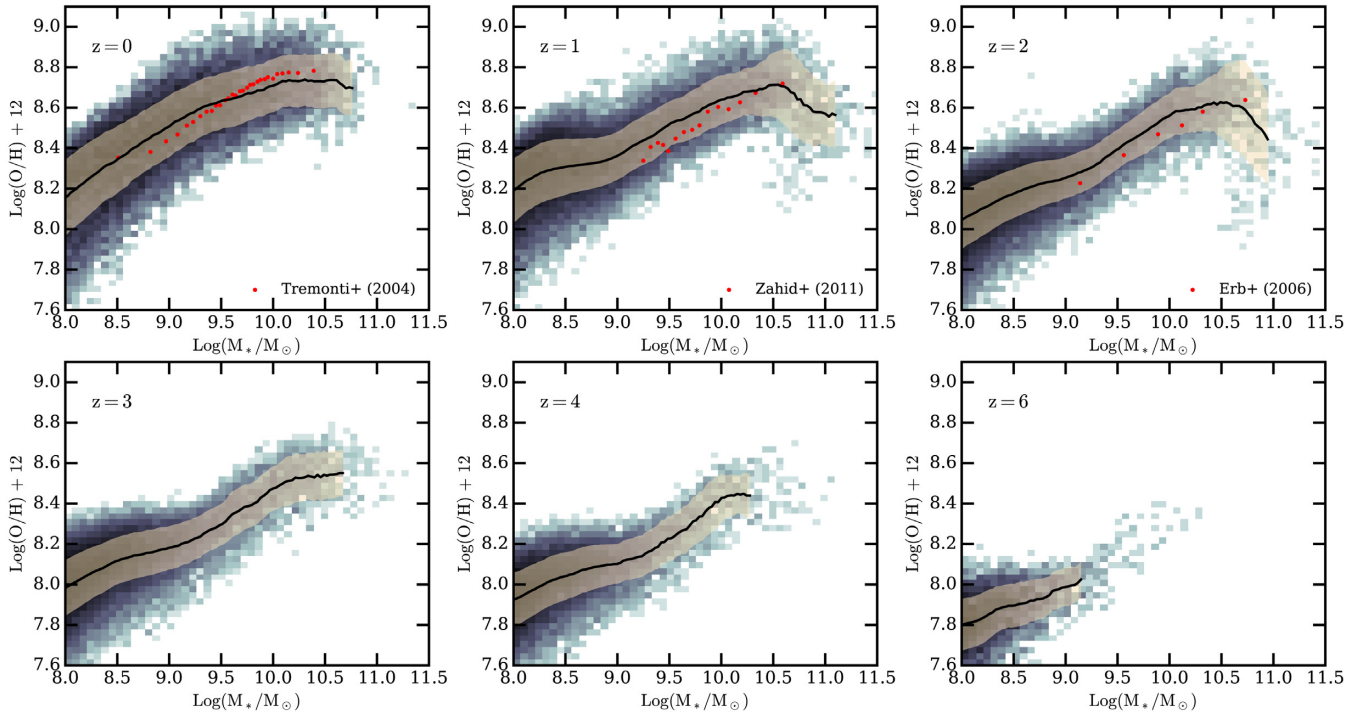


Figure 6. Gas-phase mass–metallicity relation at redshifts $z = \{0, 1, 2, 3, 4, 6\}$, as labelled in the upper left corner of each panel. The coloured two-dimensional background histogram indicates the distribution of central galaxies from the TNG100 simulation. The solid black line and surrounding shaded band indicate the median MZR and the 1σ scatter, respectively. Observational data from Tremonti et al. (2004), Zahid, Kewley & Bresolin (2011), and Erb et al. (2006) have been included in the $z = 0$, $z = 1$, and $z = 2$ panels, respectively. We do not place any emphasis on the absolute normalization of the MZR owing to uncertainties in the observed metallicity diagnostics, but instead focus on the slope and normalization evolution. Our models broadly match the low-redshift shape of the MZR and we find there is a gradual decline in the normalization with increasing redshift.

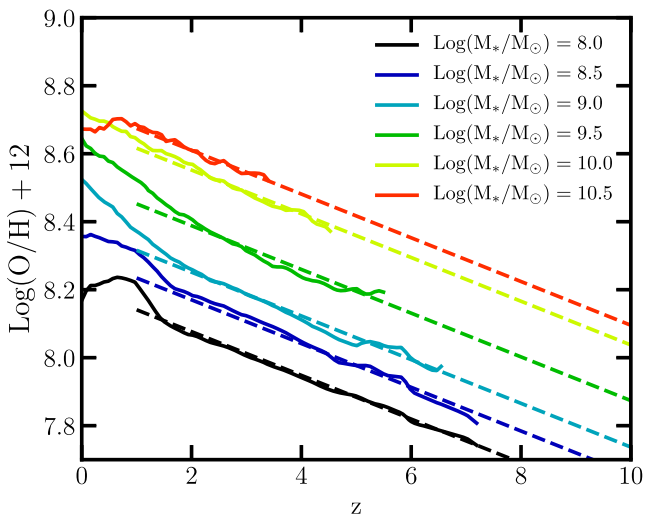


Figure 7. Evolution of galactic metallicity as a function of redshift for several mass bins, as indicated in the legend. Solid curves indicate the metallicity as determined from the simulation, while dashed lines indicate best fits and extrapolations to the data. We find a best-fitting slope of $Z \propto -0.064z$ which applies reasonably well for $z > 2$ across the full mass range resolved in our simulations.

minimization on the full dataset for $z > 1$ of $Z = Z_0 - 0.064z$. Predictions for metallicity of galaxies past $z > 6$ are dependent on the nature of our adopted extrapolation, but clearly point towards continued decline in the metallicity for all galaxy mass bins. By

redshift $z = 8$ we expect that galactic metallicity will be ~ 0.5 dex lower than redshift $z = 0$ galaxies of the same mass.

Zahid et al. (2014) argue that the existing observational MZR data out to $z = 1.55$ are accurately fit with a single, unchanging saturation metallicity. The simulated saturation metallicity, on the other hand, clearly evolves significantly as can be seen in Fig. 7 (or in Fig. 6). Importantly, however, a direct comparison of the simulated MZR relations and the data explored in Zahid et al. (2014) show that the two datasets agree reasonably well, with the strongest point of tension being whether and where one defines the saturation metallicity based on sparsely populated high-mass high-redshift data points. Our simulations agree with the Zahid et al. (2014) data in the sense that neither the simulated MZR nor the observed MZR saturation metallicity evolve significantly over the redshift range $0 < z < 1.5$, but our models do predict that there is an evolution of the MZR saturation metallicity and that this evolution will become more pronounced at increasingly high redshift. We expect that this prediction can be (in)validated in the coming years.

The driving force behind the evolution in the normalization in the MZR has been subject to widespread debate. Galactic metallicity trends with redshift or mass have been explained with competing scenarios based on changes to the metal retention efficiency or changes to the gas fractions of galaxies. Our models indicate that the ISM metal retention efficiency (which is driven by feedback) is *not* responsible for the redshift evolution of the MZR in our models. While our models indicate a decrease in the normalization of the MZR with increasing redshift, the ISM metal retention efficiency (as in Fig. 3) *increases* with increasing redshift which should give rise to an *increasing* metallicity. Changes in the ISM metal retention

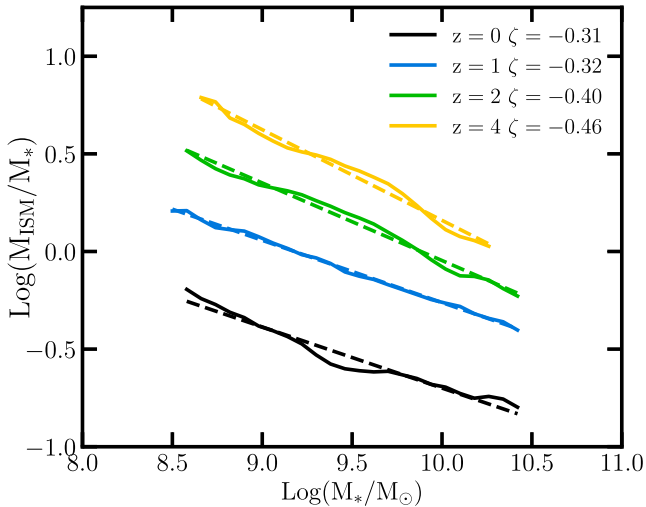


Figure 8. Gas fractions are shown as a function of stellar mass for four distinct redshifts for the simulated IllustrisTNG galaxies. We fit each redshift independently and show the slopes of the best-fitting $M_{\text{gas}}/M_* \propto M_*^\zeta$ line in the legend. Higher redshift galaxies have significantly higher gas fractions which impacts the MZR normalization evolution.

efficiencies are not responsible for the lowered MZR normalization at high redshift in our model.

Instead, the increasing gas fractions of high-redshift galaxies are the primary driver behind the redshift evolution of the MZR. Fig. 8 shows the gas fraction (defined here as M_{gas}/M_*) as a function of stellar mass for several redshifts. There are two trends present: (i) At a fixed redshift, gas fraction decays with stellar mass and (ii) at a fixed mass, higher redshift galaxies have higher gas fractions. We have found best fits to the gas fraction dependence on stellar mass using a power-law form $M_{\text{gas}}/M_* \propto M_*^\gamma$ (same as in Peeples & Shankar 2011) where the best-fitting values of γ fall in the range $\gamma = -0.3$ to $\gamma = -0.5$. In general the relation steepens with increasing redshift. The redshift $z = 0$ slope of $\gamma = -0.31$ is shallower than the published observed gas fraction values of $\gamma \approx -0.5$ (e.g. Peeples & Shankar 2011). However, this offset in slope values should be regarded with caution since the observed gas fractions are determined from, e.g. H I gas-mass measurements, which is expected to scale in the same way but is not directly comparable to the gas-mass values derived from the simulation shown in Fig. 8.

The main focus of Fig. 8 for this paper, however, is the evolution with redshift. The evolution in the gas fraction at a fixed stellar mass is significant, with gas fractions for the redshift $z = 1$ ($z = 4$) simulated galaxy population being ~ 0.5 dex (~ 1 dex) higher than the redshift $z = 0$ galaxy population. While the metal retention efficiency is increasing towards high redshift, the ISM metallicity is dropping with time, which is explained by the increasing gas fractions. This point is important to stress because some models that explain the MZR as an instantaneous competition between metal production and gas inflows do not include a dependence on gas-mass or gas fraction (e.g. Finlator & Davé 2008; Davé, Finlator & Oppenheimer 2011). For example, in the Finlator & Davé (2008) ‘equilibrium’ MZR model the gas inflow rates are assumed to exactly balance the gas consumption/outflow rates which implicitly removes the gas-mass dependence associated with predicted ISM metallicity. Our simulations clearly indicate that the evolution of gas-mass (or gas fraction) with time is the dominant

factor contributing to the MZR redshift evolution that therefore needs to be accounted for in MZR models.

4.4 The dependence of MZR scatter on gas fraction

Fig. 9 shows the median gas fraction of galaxies with respect to the MZR for six distinct redshifts. We define gas fraction in Fig. 9 as being the ratio of total gas-mass above the star formation density threshold to the total stellar mass within twice the stellar half mass radius. As has been found previously (e.g. Davé et al. 2012), there is an overall trend with mass where higher mass galaxies have lower gas fractions and that higher redshift galaxy populations have higher gas fractions when compared against their lower redshift analogues at a fixed stellar mass (as discussed in the previous subsection). However, perhaps most interesting, Fig. 9 clearly reveals the presence of a residual trend in the simulated MZR, where galaxies with high metallicities have low gas fractions, and galaxies with low metallicities have high gas fractions. The residual trend between offset from the MZR and gas fraction can be seen at all redshifts below $z = 6$. The correlation between offset from the MZR and gas fraction appears notably monotonic, with limited exceptions. Variations in the gas fraction at a fixed mass reach up to an order of magnitude in value. The continued existence of the trend between offset from the MZR and gas fraction becomes somewhat less clear at very high redshift (i.e. $z = 6$) because the volume used in the present study is simply too small to have a sufficient number of well-resolved, massive-galaxies that might allow us to continue the study of this trend. However, for the narrow mass range of $8.5 < \log(M_*/M_\odot) < 9.25$ a trend with gas fraction is still present.

Fig. 10 identifies the residual trend between scatter in the MZR and gas fraction by showing the median metallicity as a function of ISM gas-mass in thin mass bins, at several redshifts. The three panels each select galaxies in ± 0.1 dex stellar mass bins centred around $\log(M_*/M_\odot) = \{8.9, 9.5, 10.5\}$ in the left-hand, centre, and right-hand panels, respectively. Fig. 10 shows that the simulated galaxy population in IllustrisTNG displays an anticorrelation between gas-phase metallicity and ISM gas-mass, at a fixed stellar mass. A trend of this nature holds across a wide mass range. Comparing the three panels over the mass range $8.9 < \log(M_*/M_\odot) < 10.5$ shows that there is a visible increase in the average metallicity – as is expected from the MZR – while the residual trend between metallicity and ISM mass remains present but decreases in slope.

For comparison at redshift $z = 0$, the dashed red line in Fig. 10 shows the data from Bothwell et al. (2013) comparing the gas-phase metallicity versus H I gas-mass. Bothwell et al. (2013) assembled H I gas-masses from the Arecibo Legacy Fast ALFA survey (Haynes et al. 2011) and metallicity measurements from the Sloan Digital Sky Survey using the R23 parameter and $[\text{N II}]/\text{H}\alpha$ ratio as metallicity diagnostics (as applied in Maiolino et al. 2008). We note that there is significant uncertainty associated with the absolute normalization of *both* axes in this comparison. Metallicity diagnostics are known to be systematically uncertain at the $\gtrsim 0.3$ dex level (Kewley & Ellison 2008) and making a fair comparison between the observed H I gas-masses employed in Bothwell et al. (2013) and gas-masses from our simulation is non-trivial (Bahé et al. 2016; Marinacci et al. 2017a). Here we simply take the total mass of all star-forming gas in each galaxy, which likely scales with the H I gas-mass, but may underestimate the total H I gas-mass of the system. Owing to these two normalization concerns, we focus our attention on the slope of the residual correlation between metallicity and gas-mass.

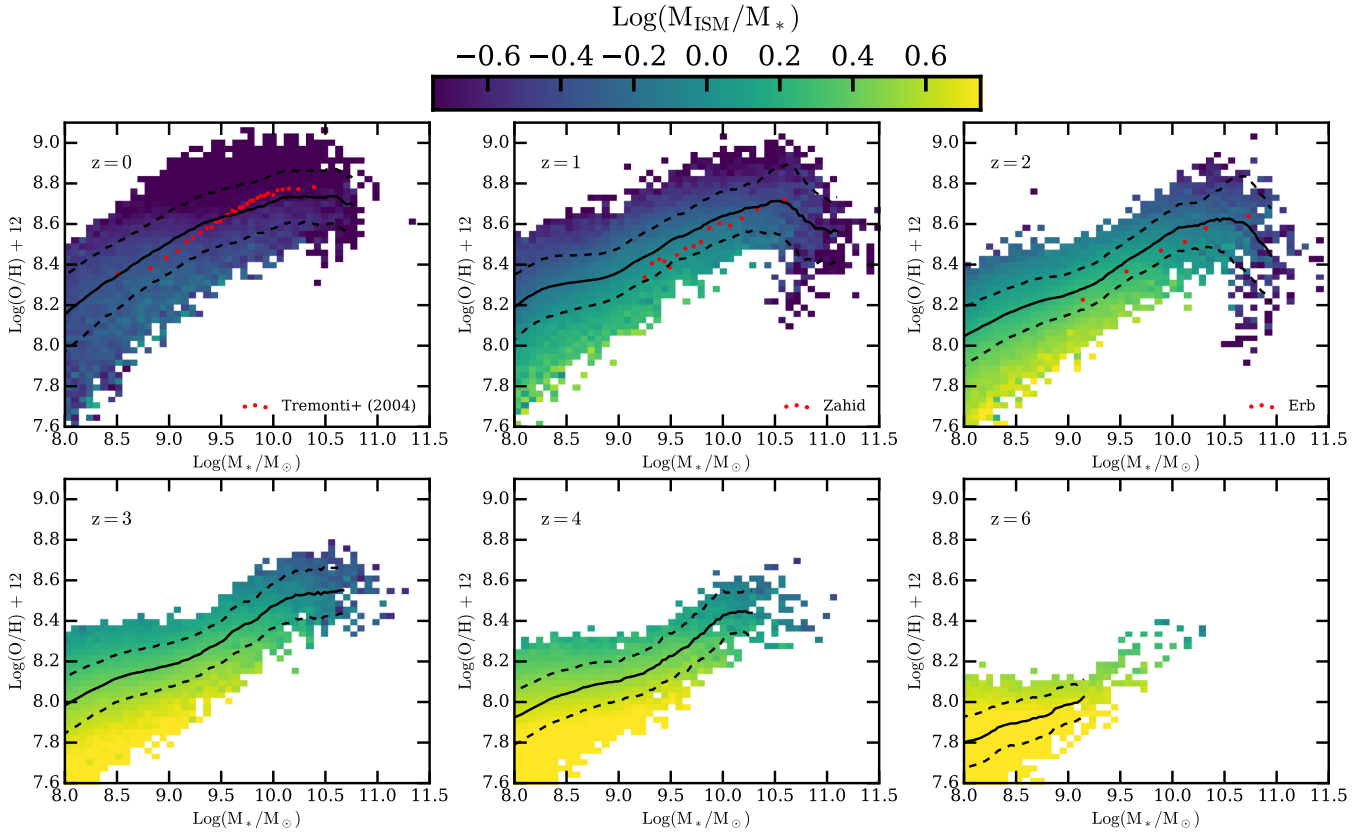


Figure 9. The median gas fraction, defined as the ratio of ISM mass to stellar mass, is shown with respect to the mass metallicity relation for six distinct redshifts as labelled in the upper left corner of each panel. As in Fig. 6, the median MZR is indicated with a solid black line, with the 1σ variation indicated with dashed black lines. A trend can be identified where galaxies with high (low) gas fractions have low (high) metallicities, when compared against the MZR. This trend holds across a wide redshift and mass range.

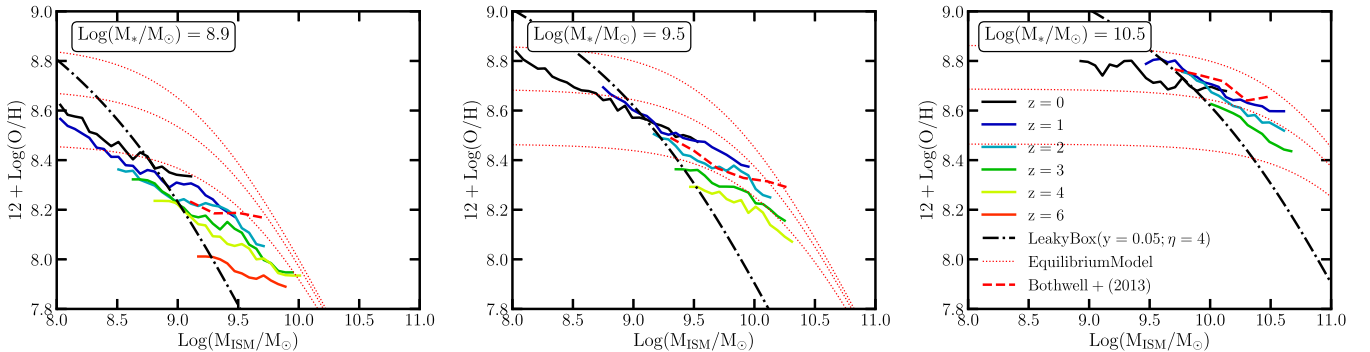


Figure 10. The average metallicity is shown as a function of M_{ISM} for three thin mass bins (corresponding to the three panels) at several redshifts as indicated within the legend. There is a clear correlation between galactic metallicity and the ISM mass where galaxies with higher ISM masses have lower metallicities. The steepness of the correlation decreases for higher galaxy mass samples. The dashed red lines indicate observational data from Bothwell et al. (2013) which broadly agrees with the simulated trends. The dot-dashed black lines indicate a leaky box model with a yield of $y = 0.05$ and an assumed outflow mass loading of $\eta = 4$. The dotted red lines indicate the equilibrium model predictions (see text for further details).

In general, the slope between metallicity and HI gas-mass found in the Bothwell et al. (2013) data is very similar to the slope found in the majority of the IllustrisTNG data between metallicity and ISM mass. In more detail, the redshift $z = 0$, low-mass IllustrisTNG galaxy metallicity (black line in the left-hand panel, in Fig. 10) scales as $Z \propto M_{\text{ISM}}^{-0.3}$, which is very similar to the Bothwell et al. (2013) trend. Moving from the lowest mass bin (left-hand panel) to the intermediate-mass bin (centre) and highest

mass bin (right) we find the continued presence of a correlation between metallicity and ISM gas-mass. However, the slope gradually flattens to $Z \propto M_{\text{ISM}}^{-0.1}$ for the highest mass bin. This slope flattening is consistent with the observed mass-dependent trend. We emphasize again, however, that some caution should be used when interpreting the exact quantitative slope comparisons between these two datasets owing to non-trivial conversions from M_{ISM} to M_{HI} .

The coloured solid lines in the three panels of Fig. 10 indicate the metallicity versus gas-mass trend found at redshifts $z > 0$. There is a gradual normalization evolution, where higher redshift galaxy populations have lower metallicities and higher ISM gas-masses at a fixed stellar and gas-mass (see also Davé et al. 2017; De Rossi et al. 2017). The slopes that describe the metallicity versus gas-mass relation are, however, nearly unchanged. Our models predict that a residual correlation between offset from the MZR and ISM gas-mass should persist in high redshift galaxy observations.

The dot-dashed black line in Fig. 10 indicates the line $Z \propto -y/(1 + \eta) \ln(M_{\text{ISM}}/(M_{\text{ISM}} + M_*))$, which corresponds a leaky box evolution track. In these plots, the employed leaky box model uses a mass loading factor for $\eta = 4$ which is numerically equivalent to a closed box model with a lowered yield of $y = 0.01$ rather than the total yield of $y = 0.05$. This outflow normalization in the leaky box is included to improve the agreement between the model and simulated data. In general, the closed box model trend is steeper than the tracks at any fixed redshift. We return to this point when discussing the connection between individual galaxy evolution tracks and net galaxy population trends in Section 5.

The dotted red lines in Fig. 10 indicate an approximate regulator model of the form (e.g. Lilly et al. 2013)

$$Z_{\text{eq}} = Z_{\text{acc}} + \frac{y}{1 + 2\eta + f_g} \quad (5)$$

where Z_{acc} is the metallicity of accreted gas, $f_g = M_{\text{ISM}}/M_*$ is the gas fraction, Z_{acc} is the metallicity of newly accreted material, and η is the wind mass loading factor. To facilitate the comparison in Fig. 10, we assume $Z_{\text{acc}} = 0$, $y = 0.05$, and $\eta = \{0.5, 1, 2\}$. While holding the wind mass loading fixed, the equilibrium model lines are described by two limiting behaviours in the gas rich, $Z \propto yM_*/M_{\text{ISM}} \propto M_{\text{ISM}}^{-1}$ and gas poor, $Z \propto y/(1 + 2\eta)$, regimes. As with the closed or leaky box model, the regulator model is not a very compelling fit to the simulated data. We generally find that the regulator model is too steep at high-ISM mass values, and too shallow at low-ISM values.

As discussed in detail in Section 5.1, the steepness of the slope seen in Fig. 10 is set by movement of individual galaxies as they undergo periods of metallicity dilution via metal-poor gas accretion from the CGM and metal enrichment via star formation (Genel 2016). There are two primary factors that we observe as influencing the flatter residual trend among high-mass galaxies. First, higher mass galaxies tend to have lower gas fractions, which results in flatter closed/leaky box model evolution tracks.⁴ Secondly, higher mass galaxies have increasingly enriched CGM gas reservoirs, which reduces the impact of metallicity dilution via gas accretion.

A number of observational papers had previously identified residual correlation between offset from the MZR and galaxy SFR (Ellison et al. 2008a; Lara-López et al. 2010; Mannucci et al. 2010). Although we do not show it here, a very similar residual trend between ISM metallicity and SFR is also found in our simulations (see e.g. Fig. 11 and Torrey et al. 2018). We omit showing this result because it is qualitatively identical to that presented in Fig. 10 and the ISM gas-mass is a more direct driver of ISM metallicity since it directly enters into the metallicity determination.

5 RESULTS: TIME EVOLUTION OF GALAXIES

In this section we explore how galaxies evolve with respect to the MZR. Fig. 11 shows two detailed examples of how galaxies evolve in time including their gas distribution (top postage stamps), metallicity (top time series), SFR (second row), ISM mass (third row), and the rate of change of ISM mass (bottom row) over a period of a few (~ 3) Gyr starting at low redshift. The evolution tracks have been shaded with red and green to indicate periods of time when the ISM is net increasing or decreasing in mass, respectively. Changes to the ISM mass can be driven by inflows, outflows, star formation, or stellar mass return. The dashed line in the metallicity evolution time series indicates the mean value for the MZR for a galaxy at that mass and redshift. The two systems presented in Fig. 11 are not particularly special, but were selected because (i) they reside within one of the ‘subboxes’ in the IllustrisTNG simulation that has high time frequency snapshot output and (ii) they highlight some of the diverse physical mechanisms that can drive galaxy metallicity evolution.

The left-hand panel of Fig. 11 features a relatively low-mass system, with a stellar mass of $M_* \approx 10^9 M_\odot$. This system spends most of its early evolution with a metallicity at or below the MZR, which changes very close to redshift $z = 0$. There are two notable galaxy merger events (both with mass ratio 1:3 or greater) which occur for this system at $z \approx 0.08$ and $z \approx 0.15$ (these times have been marked in the figure using vertical thin black dashed lines) that both have easily identifiable impacts on the metallicity, SFR, and ISM mass. Leading up to the merger event, there is an easily identifiable influx or increase of ISM mass which coincides with the decreases in the ISM metallicity owing to metallicity dilution, and increases in the SFR. This is the same physical picture that has been found in idealized galaxy merger simulations (Scudder et al. 2012; Torrey et al. 2012a; Patton et al. 2013) and which is supported with observations of close pair galaxies (Ellison et al. 2008b; Rich et al. 2012; Scudder et al. 2015). Outside of these two discrete events, the metallicity evolution of this system is not described by a single coherent physical picture. The system undergoes periods of time of perpetuated metallicity increase (e.g. from $0.175 < z < 0.225$) which are broadly associated with sustained high levels of star formation activity, but the system also undergoes periods of time of sustained metallicity decrease (e.g. from $0.225 < z < 0.275$) which are not immediately qualitatively distinct from periods of metallicity increase.

The right-hand panel of Fig. 11 is similar to the left, but features a relatively massive galaxy, with a stellar mass of $M_* \approx 10^{11} M_\odot$. In contrast to the left-hand panel, this system does not undergo any significant merger activity over the observed period but is actively experiencing AGN feedback. The impact of AGN feedback can be seen clearly through the change in the gas distribution between the rightmost and second-to-right gas distribution where a central gas cavity is created and sustained. The central low-density gas cavity is created by removing the central – highest metallicity – gas from the ISM. This drives a sharp drop in the central gas metallicity that can be observed around $z \approx 0.26$ (Nelson et al. 2018b). After this drop, the metallicity evolution of this system is reasonably constant, while the ISM mass and SFRs drop rather continuously from redshift $z = 0.2$ to $z = 0$.

One of the main points to take away from Fig. 11 is that the metallicity evolution of galaxies is governed by a somewhat subtle competition between gas inflows, gas outflows, and metal enrichment. We can assert that periods of metallicity decrease are associated with dominant contributions of influxes of lower

⁴We show in Section 5.1 that galaxies regularly follow leaky box model trajectories for limited portions of their evolution.

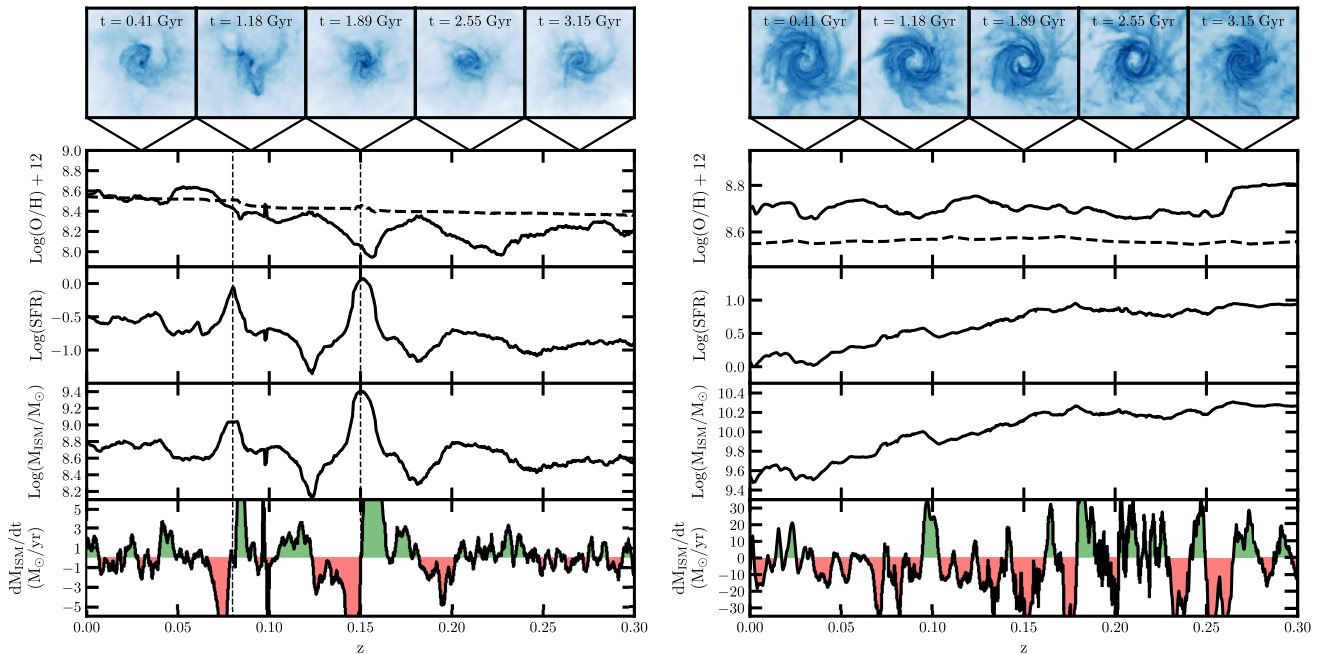


Figure 11. Example evolution tracks for two galaxies are shown. The top postage stamp images indicate the gas-mass distribution at five times. The bottom time series indicates the evolution of the ISM metallicity, SFR, ISM gas-mass, and net rate of change of ISM gas-mass. The dashed line in the metallicity evolution time series indicates the mean value for the MZR for a galaxy at that mass and redshift. The system in the left-hand panel is lower mass ($M_* \approx 10^9 M_\odot$) than the system on the right ($M_* \approx 10^{11} M_\odot$). The system on the left undergoes two mergers which are indicated with vertical dashed lines.

metallicity gas to the ISM or ejections of high-metallicity ISM. However, outside of merger events the magnitude of gas inflows on to the ISM is set by subtle changes to the ambient CGM properties which itself can be impacted by recent accretion activity, recent outflow activity, feedback from the AGN, or environmental interactions. This demonstrates the core difficulty associated with modelling galaxy individual metallicity evolution analytically: galactic metallicity evolution is highly variable and dependent on a number of rapidly varying factors.

5.1 Characterizing individual ism metallicity evolution tracks

To further probe the nature of the metallicity evolution tracks that galaxies follow, Fig. 12 shows evolution tracks in metallicity versus ISM mass space for 10 individual galaxies tracked in time using SUBLINK (Rodríguez-Gomez et al. 2015). For clarity of discussion, each panel is labelled with a number in the lower left corner. Evolution tracks in Fig. 12 can help diagnose the relative importance of inflows/outflows – which will have a direct impact on the ISM mass – versus star formation and chemical enrichment. The evolutionary tracks within each panel are coloured to go from red at $z = 0.35$ to blue at $z = 0$. The dashed black line indicates a leaky box model line of $Z = -y/(1 + \eta) \ln(M_{\text{ISM}}/(M_{\text{ISM}} + M_*))$ where we adopt a yield of $y = 0.05$ and outflow mass loading of $\eta = 4$. The leaky box model is evaluated separately for each system at a fixed stellar mass of $M_* = M_*(z = 0)$ – which is a reasonably good approximation for most of the systems shown over the plotted redshift range.

The first point to take away from Fig. 12 is that galaxies can move in any direction in metallicity versus ISM space. Each galaxy has a truly unique track which is, in general, non-monotonic both in terms of ISM mass evolution and metallicity evolution. There is a slight preference for galaxies to move along the diagonal direction from

upper left to lower right, similar to the orientation of the closed or leaky box model. However, there is not a single coherent evolution track or pattern visible in this space.

However, there are some regular features identifiable in Fig. 12 from the individual galaxy metallicity evolution tracks. One such trend is that there are identifiable periods of time where individual galaxies closely follow leaky box model evolution tracks. For example, panels 2, 8, and 9 all feature galaxies that evolve along, or directly parallel to, the closed box model for a Gyr or longer. Closer inspection of these systems reveals that they are evolving similarly to the leaky box style model tracks because they are in relative isolation, with modest or low accretion rates on to the ISM, and strong ongoing star formation. The presence of leaky box model behaviour is very notable since these galaxies are evolving in a fully cosmological environment with time-variable inflows and outflows consistently perturbing the system. While the role of outflows may be captured with our employed leaky box model, there are many other effects that such as fluctuations in the gas inflow rates, variable inflow/outflow gas metallicity, merger events, internal bar/galaxy instabilities, etc. all of which can impact the ISM metallicity evolution.

Systems are driven off leaky box model tracks by rapidly changing the properties of the ISM gas reservoir. The ISM gas reservoir can be perturbed by merger events (as was demonstrated in Fig. 11). However, we find that most of the non-closed- or non-leaky box model evolution is more subtle in nature and not associated with distinct merger events. We find that perturbations to the central gas disc and outflows associated with feedback are the two primary drivers of non-closed- or non-leaky box model behaviour. Bars or clumps that form in the central gas disc have the ability to perturb an otherwise stable system, which can cause the central gas disc to torque down the gas around it. When this occurs, the central gas density rises and the ISM mass increases, forcing

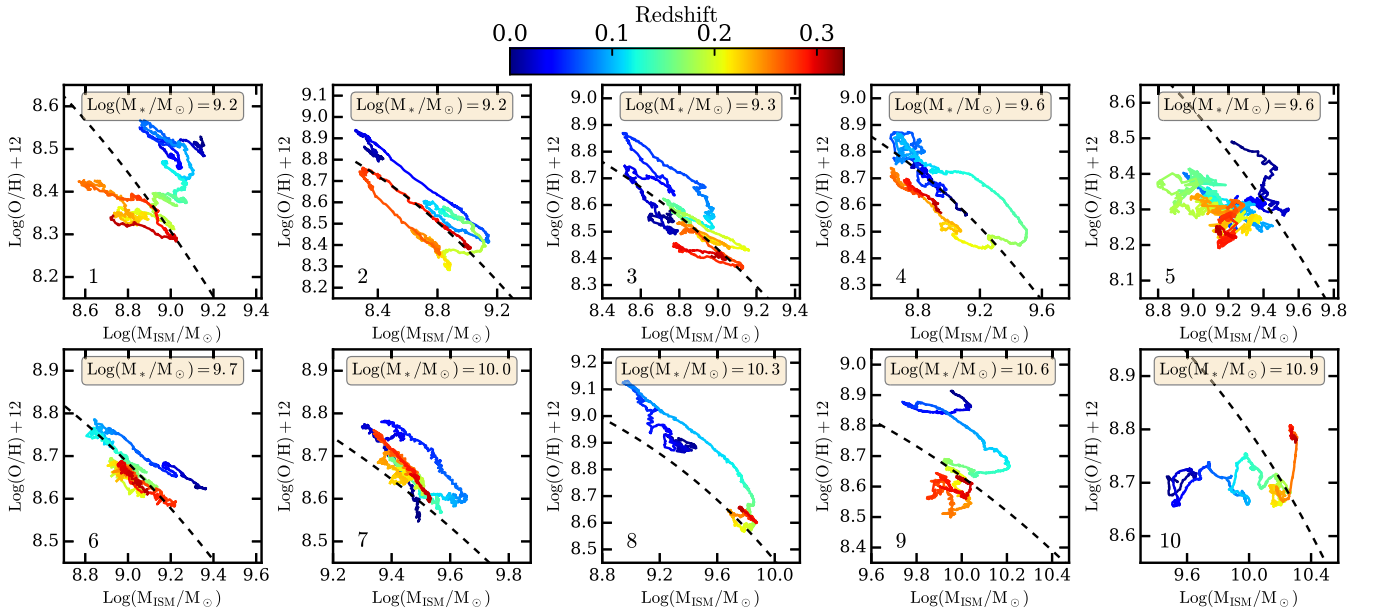


Figure 12. Evolution tracks of metallicity and ISM mass are shown as a function of time for 10 individual galaxies. Tracks in each panel show the evolution from $z = 0.35$ (in red) to $z = 0$ (in blue). The black dashed lines indicate leaky box model evolution tracks where we have used a yield of $y = 0.05$ with an outflow mass loading factor of $\eta = 4$. Redshift $z = 0$ stellar masses for each system are indicated within each plot. The number in the lower left corner of each panel is assigned for ease of identification.

systems to the right in Fig. 12. At the same time, this process of gas inflow/accretion can dilute the ISM metallicity depending on the metal content of the newly acquired ISM material. The behaviour is demonstrated, e.g. at early times in panel 6, intermediate times in panel 2, or late times in panel 4.

Outflows, on the other hand, predominately function to drive down the ISM mass. Panel 10 of Fig. 12 shows the same system featured in the right-hand panel of Fig. 11 which is dominated by AGN feedback over the time period shown. As a result of the AGN feedback driving out ISM material, this system gradually moves towards lower ISM masses without very systematic or strong changes to the ISM metallicity.

The central complication with deciphering the evolution tracks in Fig. 12 is that – while there are periods of clearly understood evolution driven by distinct physical mechanisms – much of the evolution of these systems is dominated by a combination of multiple effects. In general, systems are experiencing accretion on to the ISM, star formation, enrichment, and outflows simultaneously. It can be broadly argued that in many cases galaxies appear to oscillate between accretion driven movement to the lower right, followed by star formation and enrichment dominated movement to the upper right. However, any claim along these lines requires a more statistical characterization of the distribution and movement of galaxies in this space.

5.2 Characterizing statistical ISM metallicity evolution trends

Fig. 13 shows the net distribution and evolution for an ensemble of galaxies in metallicity versus ISM mass space. Each panel shows a two-dimensional histogram indicating the distribution of galaxies as well as a series of vectors indicating the average evolution direction and speed for galaxies in this space. The distribution of galaxies is shown at redshift $z = 0.058$, and the evolution direction and speed is calculated by tracking each galaxy forward to $z = 0$. The average evolution direction and speed is taken to be the mean ISM mass

change and mean metallicity change for all galaxies residing in each pixel. Arrows are only indicated for pixels containing at least five galaxies.

For the lowest mass bin (upper left) a clear anticorrelation can be seen between the ISM metallicity and ISM mass with galaxies with higher ISM masses having lower ISM metallicities. Examining the vector distribution we find that galaxies are moving back towards a central ISM mass and ISM metallicity value from both ends of the distribution when averaged over the full population. This restoring movement can be interpreted based on the evolutionary tracks explored in Figs 11 and 12. Galaxies sitting in the lower right portion of this plot which have large ISM gas-masses have large SFRs (see Fig. 11) and are therefore most likely to be enrichment dominated and possibly moving along leaky box model type trajectories (as demonstrated in Fig. 12). The right portion of the plot has been shaded yellow to indicate this ‘enrichment dominated’ portion of the galaxy population. Conversely, galaxies in the upper left portion of this plot have comparatively low-ISM masses, comparatively low SFRs, and therefore comparatively low enrichment rates. However, the low-ISM gas-mass reservoirs in these systems make them particularly susceptible to influence from gas inflow events. The restoring force for galaxies in the upper left portion of this plot is accretion of new gas from the CGM, which will simultaneously drive the ISM to lower metallicities and higher ISM masses. The left portion of this plot has been shaded green to indicate the regions where the ISM mass and metallicity evolution is accretion dominated.

Similar trends can be seen for the upper-right and middle-left panels, which display higher mass bins. There are clearly identifiable trends for galaxies in the enrichment and accretion dominated regimes, although the median ISM mass and metallicity for the overall population shifts to somewhat larger values with increasing galaxy mass. These trends, however, become less clear as we move to the middle-right and bottom panels, which display the two highest mass bins. In the bottom panel, we find that there is

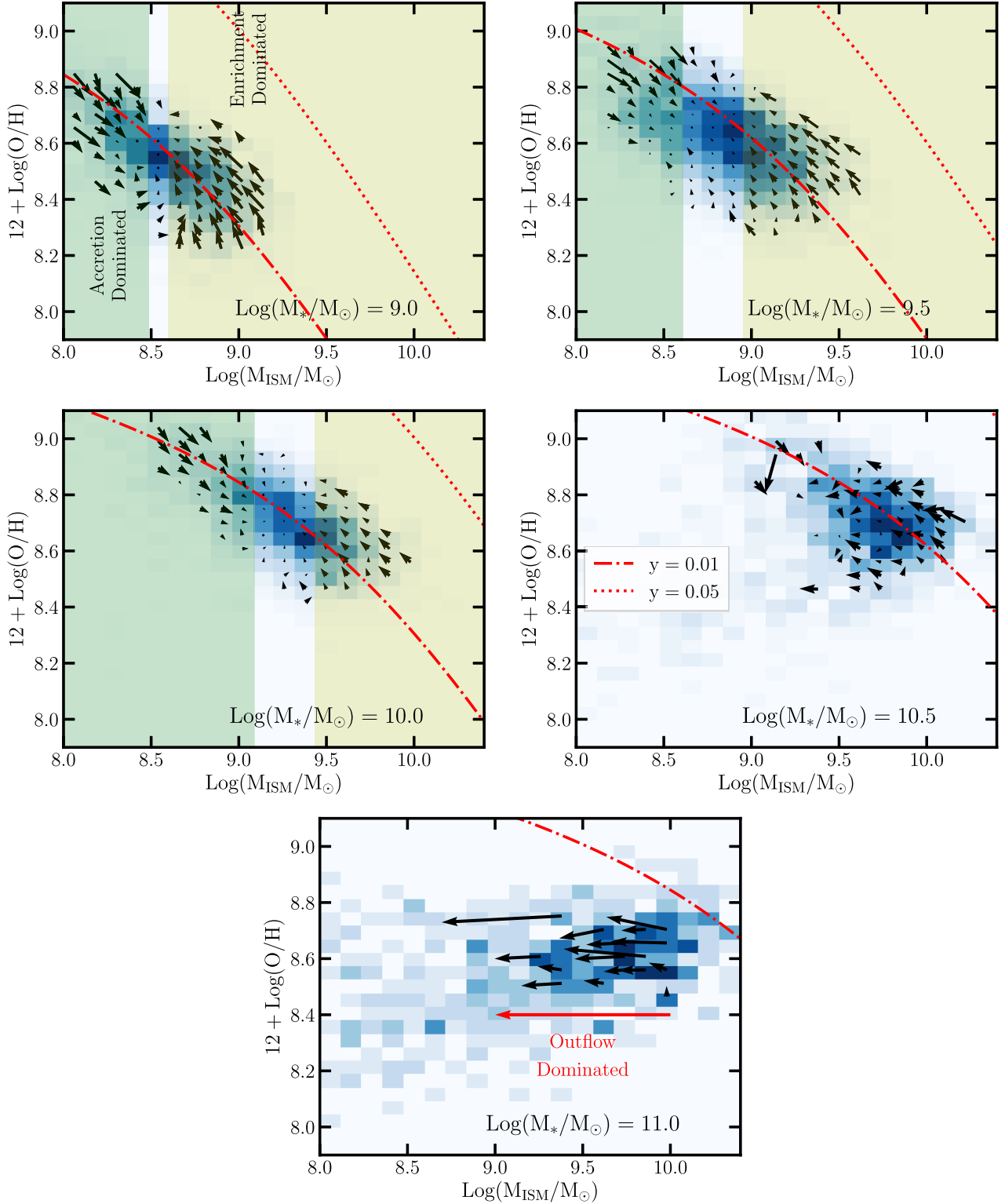


Figure 13. The distribution and evolutionary trends of galaxies in metallicity versus ISM mass is shown for several stellar mass bins, each of width ± 0.25 dex. The background two-dimensional histograms indicate the distribution of galaxies at $z = 0.058$, while the vectors indicate the average evolution direction and speed within this space calculated by tracking galaxy movement over the redshift range $0 < z < 0.058$. Clear patterns can be identified for the movement of galaxies in the lowest three mass slices. The first three panels (lowest three mass slices) include green and yellow colour coded regions which indicate regions in this space where galaxies are predominately evolving owing to fresh gas accretion and star formation driven enrichment. In contrast, the bottom panel (highest mass bin) includes only a single arrow pointing to the left which indicates the direction galaxies move when they are outflow dominated. All panels show also leaky box model tracks with yield of $y = 0.05$ and an outflow mass loading of $\eta = 4$ (red dot-dashed line) and $\eta = 0$ (red dotted line; equivalent to a closed box model).

not a visible residual trend between ISM mass and metallicity and galaxies are moving horizontally to the left. This trend for these highest mass galaxies is dominated by AGN-driven outflows which drive down the ISM gas-mass without significantly diluting or enriching the ISM metallicity. The middle-right panel is a transitional population of galaxies, which shows some indication of accretion and enrichment, but where the trends are less pronounced owing to the influence of an increasingly impactful AGN contribution.

6 DISCUSSION

In this paper we have provided a top-down examination of the metal distribution and evolution for the TNG100 galaxy formation simulation. As in the original Illustris simulation, the IllustrisTNG feedback model was refined predominately based on matching stellar mass functions and the cosmic SFR density (black hole mass to galaxy or halo mass relation, halo gas fractions, and galaxy sizes were also considered; Weinberger et al. 2017; Pillepich et al. 2018b). The stellar and AGN feedback that was employed was tuned to help galaxies regulate their stellar mass growth accordingly. However, the same feedback that is used to regulate the stellar mass growth of the simulated galaxy population has a distinct impact on the distribution of metals in-and-around galaxies. Examining the metal distribution is therefore an interesting test of the model as it is both independent of the core constraints used to tune the IllustrisTNG model, and sensitive to the feedback strength and implementation. In this section, we aim to synthesize our results into a clear and coherent theoretical picture, discuss how this work contributes to or addresses outstanding questions surrounding the coevolution of galaxies and their metal content, and identify some implication of our analysis.

6.1 What do metal retention efficiencies physically tell us about the MZR shape?

Our analysis indicates that the average ISM metal retention efficiency is very similar for the galaxies across the mass range $10^9 < M_*/M_\odot < 10^{10}$ (see the left-hand panel of Fig. 3). Generally, galaxies with stellar masses below $M_* < 10^{10.5} M_\odot$ have metal retention efficiencies of order ~ 0.005 at redshift $z = 0$, and with a very similar (i.e. mass independent) redshift evolution trend. Given our definition of the metal retention efficiency in equation (2), we can express the ISM metallicity as $Z_{\text{ISM}} = \gamma_{\text{ISM}} f_g$. Since we have measured the metal retention efficiency at several mass scales and found that there is limited mass dependence to the metal retention efficiency below this stellar mass threshold, this directly indicates that the low-mass-end MZR slope in our model is almost exclusively set by changes in galactic gas fraction with galaxy mass in the context of our retained metal yield framework. By examining the redshift $z = 0$ (black line) gas fraction versus stellar mass relation of Fig. 8 a clear trend can be seen of decreasing gas fraction with increasing galaxy stellar mass. The lower gas fractions of higher mass galaxies are responsible for driving the low-mass end MZR slope in the IllustrisTNG model when using our retained metal yield framework.

However, it is important to note that the retained metal yield itself depends both on the amount of metals that were ejected, as well as the amount of metals that were locked into stellar populations. The ISM metal-mass can be expressed as $M_{Z,\text{ISM}} = M_{Z,\text{total}} - M_{Z,\text{eject}} - M_{Z,*}$, where $M_{Z,\text{eject}}$ is the amount of metals ejected from the combined ISM and stellar phases and $M_{Z,*}$ is the metal-mass locked into stars. As the stellar mass and metallicity of a galaxy increases,

the amount or fraction of metals that are locked into stars also increases. This means that a constant retained metal yield does not imply a constant metal ejection rate, efficiency, or total mass. To the contrary, since the absolute mass or fraction of metals locked into stars generally increases with increasing galaxy mass (see e.g. Table 1, but also the closed or leaky box model results), the amount of mass ejected from the combined ISM plus stellar phases of low-mass galaxies must adjust in order to accommodate the nearly constant metal retention yield that we measure in our simulations. Indeed, looking at Table 1, we find that the total amount of metals ejected from the ISM and stars combined is greater for lower mass galaxies. This is consistent with the fact that lower mass galaxies have higher mass loading factors in IllustrisTNG.

We note that our conclusions for what drives the shape of the low-mass end of the MZR is difficult to judge against ‘bathtub’ or ‘equilibrium’ model analyses. For example, in the Finlator & Davé (2008) bathtub style model – which can successfully reproduce the shape and slope of the MZR under varied assumptions about outflow/feedback properties – the gas inflow rates are assumed to exactly balance the gas consumption/outflow rates such that $\dot{M}_{\text{acc}} = (1 + \eta)\dot{M}_*$. The resulting predicted MZR has a slope of $Z_{\text{bathtub,eq}} \propto \eta/(1 + \eta)$ which is set by a competition between inflows, enrichment, and outflows, where the mass dependence of the wind mass loading factor, η , ultimately sets the slope. Physically, this has been interpreted as indicating that lower mass galaxies have lower metallicities because they are much more efficient at removing metals from the ISM. This interpretation appears to be in conflict with the results presented in Fig. 3 because if we consider only the ISM material, our models indicate that low-mass galaxies (i.e. $M_* \sim 10^9 M_\odot$) are similar – or marginally more efficient – at retaining their metals in their ISM when compared against higher mass (i.e. $M_* \sim 10^{10} M_\odot$) systems. However, if we instead consider the retained metal yield for both the ISM and stellar components – leaving out only the outflow component – we find that low-mass galaxies are somewhat more efficient at ejecting metals ($\gamma_{\text{ISM}} + \gamma_* = 0.015$ for $M_* \sim 10^9 M_\odot$, implying $\gamma_{\text{outflow}} = 0.35$) than their higher mass companions ($\gamma_{\text{ISM}} + \gamma_* = 0.02$ for $M_* \sim 10^{10} M_\odot$, implying $\gamma_{\text{outflow}} = 0.3$). In this sense, our IllustrisTNG model qualitatively agrees with the bathtub models in asserting that lower mass galaxies use outflows to expel a somewhat larger fraction of their metals than their higher mass companions.

Quantitatively, however, we note that this ~ 10 per cent change in γ_{outflow} is insufficient to explain the factor of ~ 2 change in the metallicity between $M_* \sim 10^9 M_\odot$ and $M_* \sim 10^{10} M_\odot$ systems. In order to explain the slope of the MZR, our analysis requires a strong relationship between gas fraction and galaxy mass which dominates the slope determination. This conclusion is qualitatively different from the bathtub model given that there is no gas fraction dependence in the bathtub model MZR slope calculation. Reconciling the apparent successes of the bathtub model with the apparent tension with our explicitly calculated metal retention efficiencies is best done by considering the assumptions required to analytically model galactic metallicity evolution. In particular, it is very difficult to appropriately model the time- and mass-dependent recycling of winds, which directly impact the galactic gas- and metal-mass evolution. The assumption that winds are launched with the average galactic metallicity and never return is a strong assumption which does not fit the IllustrisTNG galaxies well.

We note that the same core challenge/problem exists for equilibrium models. The main difference between bathtub and equilibrium models is that both the gas-mass and metal-mass are time variable. As a result, the general predicted equilibrium metallicity within the

regulator models (equation 5) has an explicit gas-mass dependence. Although allowing time-variable gas-masses results in an informative link being formed between the equilibrium metallicity and the galaxy’s gas fraction (which our analysis suggests is important) the same core challenge exists for equilibrium models: the magnitude and time-scale of gas wind recycling is analytically unconstrained, and poorly accounted for in the standard formulation. In particular, one can imagine a situation where the mass loading factor is large, but the wind recycling time is very short (compared to any relevant time-scales, for the sake of example). In that situation, metals would not be efficiently carried away from the ISM in winds owing to the short wind recycling time-scales. Instead, any metals removed from the ISM will quickly return. This re-accretion of wind material could possibly be absorbed into a lowered efficiency factor preceding the wind mass loading, or possibly by modifying the metallicity of accreted gas Z_{acc} . However, building a predictive analytic link between the wind mass loading factor, wind metallicity, wind recycling time, cosmic accretion rate, and accreted gas metallicity is not straightforward.

The fact that the shape of the IllustrisTNG MZR is dominated by the mass-dependent gas fractions – and not the efficiency with which metals are ejected via outflows – is an important conclusion of the analysis in this paper. The evidence for this conclusion is that – despite mass-dependent wind mass loading factors – the ISM metal retention efficiency is nearly invariant across the mass range $10^9 < M_*/M_{\odot} < 10^{10.5}$. This may indicate that the limited accounting for recycling of wind material in bathtub and equilibrium analytic models of the MZR has led to an overestimation of the relative importance of metal ejection via outflows in setting the shape of the MZR. This suggestion needs to be checked by alternative galaxy formation models, which can be done by directly measuring the metal retention efficiency as a function of galaxy mass as presented in Fig. 3.

6.2 Testing galaxy feedback models with metallicity

Although metals are produced via stars that formed from dense gas, the majority of metals live outside of the ISM. We demonstrated the strong redistribution of metals through global (Fig. 1) and galactic (Fig. 2) phase diagrams, as well as by tabulating the ‘retained metal yield’ for the ISM, CGM, and stars. Some of the metal redistribution can be driven by naturally occurring galaxy dynamics including galaxy mergers and interactions, but feedback likely plays a significant role in metal redistribution. Feedback pumps metal enriched gas out of the dense ISM into the hot/diffuse CGM around galaxies and is able to eject some fraction of metals out of their haloes all together. The metal yields quoted in Table 1 show a significant fraction (~ 10 – 20 per cent) of a galaxy’s metal content has been ejected from the halo, across a wide mass range. The fraction of ejected metal-mass increases for massive haloes to ~ 50 per cent, which is driven in part by the increased impact of AGN feedback (Nelson et al. 2018b; Weinberger et al. 2018). In our model, high-mass galaxies are more efficient at ejecting their metal-mass compared with their low-mass counterparts (see Figs 2 and 3 and associated discussion in Section 3.2).

Although the central focus of this paper has been on the MZR and metal content of the ISM of galaxies, the widespread distribution of metals make observations of *both* the ISM metallicity (e.g. through nebular emission line measurements) *and* CGM metal content (e.g. through quasar absorption line studies) critical towards understand the coevolution of galaxies and their metal content. The MZR found in our simulations scales reasonably well with current

observational constraints. However, this does not imply that the IllustrisTNG model is a unique ‘correct solution’ to how the MZR is shaped and evolves with redshift. To the contrary, the observed shape and evolution of the MZR has been recovered by other groups using models with significantly different galaxy formation models (Finlator & Davé 2008; Davé et al. 2011, 2017; Torrey et al. 2014; Ma et al. 2016; De Rossi et al. 2017). As we have argued previously, there is a degeneracy between the ISM metal retention efficiency and changes in galactic gas fractions as a function of mass and redshift. This degeneracy can be in part broken by (i) considering more careful comparisons of the galactic gas fractions and/or (ii) comparing the total metal reservoir found in the CGM against observations (e.g. Nelson et al. 2018b).

We note the trend found in our models as a function of redshift for the hot CGM metal retention efficiencies found in Fig. 3 indicate a slow redshift evolution, changing only by a factor of ~ 2 out to high redshift. This is likely a product of our wind feedback modelling, which itself is only a weak function of redshift. The slowly evolving hot CGM metal retention efficiency does not necessarily imply a slowly evolving metallicity nor slowly evolving covering fraction for any particular species. Instead, it simply implies that the hot CGM in our models hosts a fraction of the total metal budget that slowly evolves. Comparisons with metallicity and/or covering fraction calculations would require further knowledge of the total CGM gas-mass (i.e. how much pristine gas the enriched gas is diluted among) and halo size (Nelson et al. 2018b).

The sensitivity of the metal redistribution to the presence of feedback makes the effective yields discussed in Section 3 important predictions that should be checked against other theoretical models and observations, where possible. We expect that a more careful examination of the global metal budget could reveal areas of more clear tension between the IllustrisTNG results and observations, which may point to areas where feedback modelling may need to be modified.

6.3 Is there a fundamental metallicity relation?

The existence, or lack of existence, of a fundamental metallicity relation has been a point of contention in the literature (e.g. Kashino et al. 2016; Telford et al. 2016). It remains unclear whether the initial claims about correlated scatter about the MZR are a fundamental property of galaxies (Salim et al. 2014; Brown et al. 2018), or whether these correlations are driven by observational systematic biases in metallicity determinations (Sánchez et al. 2013; Barrera-Ballesteros et al. 2017). This debate will likely continue as methods of metallicity determination are refined and larger high-redshift galaxy datasets are obtained (e.g. Maier et al. 2014; Steidel et al. 2014). Using our simulations, however, we can discuss the physical motivation for the fundamental metallicity relation.

We find clear evidence in our models for the existence of a correlation between the scatter in the MZR and galactic gas-mass (see Fig. 9). A similar correlation exists between the scatter in the MZR and galactic SFR. We explored the role that gas-mass – not SFR – plays in explaining scatter about the MZR because the increased (decreased) SFRs follow as a consequence of the increased (decreased) gas-masses.

This existence of correlated scatter about the MZR persists out to high redshift, with limited changes in the slope of the correlated scatter (see Fig. 10). The slope of the correlated scatter flattens with increasing galaxy mass, which is driven by a combination of (i) increasing metallicity of accreted gas and (ii) a flattening of the slope of closed- or leaky box model evolution tracks at low gas fractions.

We stress that galaxies do not evolve along any single ‘fundamental’ metallicity plane, but instead follow unique tracks which are shaped by the accretion, merger, and star formation history of every galaxy individually (see Fig. 12). There are often repeated trends which are identifiable in the individual galaxy evolution tracks including periods of evolution along leaky box model trajectories and periods of evolution along accretion driven trajectories. We also note, however, that the presented median relations are somewhat subject to how we have fit the median of this two-dimensional distribution. In our analysis, we have simply taken the median metallicity as a function of gas-mass, which may yield a slightly different result when compared against a different bisection method. This may impact the detailed strength of the derived slope, but will not impact our qualitative conclusions.

When we average over the full galaxy population (see Fig. 13), we find that coherent trends emerge among the movement of galaxy populations about the MZR. Specifically, there is a coherent effective ‘restoring force’ that constantly operates to bring galaxies back towards an equilibrium metallicity and ISM mass. We argued that – based on inspection of a large number of individual galaxy evolution tracks – this can be physically explained as a competition between periods of gas-rich, enrichment domination and periods of gas-poor, accretion domination. Galaxies with high gas-masses have accordingly high SFRs, which increases the likelihood that galaxies move along leaky box model style trajectories. Conversely, while galaxies with low gas-masses are not necessarily more likely to be accreting rapidly, their gas accretion time-scales (i.e. $\tau_{\text{acc}} = M_{\text{ISM}}/\dot{M}_{\text{acc}}$) are shorter than their gas rich counterparts for a fixed accretion rate. These systems are therefore more likely to be accretion dominated.

In our models, the MZR emerges as a consequence of natural variability in the accretion and enrichment histories of galaxies. Variability is seeded by natural fluctuations in the accretion history of each galaxy which itself is a result of the cosmic environment in which the galaxy evolves. Forbes et al. (2014) presented a regulator-style model similar to that of Lilly et al. (2013), but with the relaxed assumption that $dZ/dt \neq 0$. They showed that variability in the galactic gas accretion history can drive correlated scatter about the MZR using a combination of analytic modelling and Monte Carlo simulations of galaxy growth tracks. The spirit of the model and results presented in Forbes et al. (2014) is in agreement with our simulations, with one subtle exception. Forbes et al. (2014) link variability in the ISM accretion rate to variability in the halo accretion rate. While this is likely in part true, we would argue based on inspection of our simulated galaxy sample that a significant fraction of the ISM mass accretion rate variability is driven by internal galaxy dynamics and the boundary conditions at the disc–halo interface. This can be important because Forbes et al. (2014) required scatter in the halo accretion rates that was in tension with (smaller than) N-body simulations in order to match the correlated scatter about the MZR. Effectively, the CGM can act as a variability damper such that the accretion on to the ISM from the CGM can contain lower amplitude and frequency variations compared to the halo accretion rates.

The IllustrisTNG model does contain one variable (the wind metal loading factor) which can impact the overall normalization of the ISM metallicity. However, there are not any *direct* parameters that would allow us to impact or tune the presence or slope of the residual correlation between the scatter about the MZR and galactic gas fractions. Given the clear presence and persistence of this residual correlated scatter in our models as well as the presence of a clear and simple physical picture for the driving of the correlated

scatter, we expect that this trend should be observable. Based on our simulations and analysis, we expect that as methods for calculating metallicity from nebular emissions lines continue to be refined and as high redshift galaxy metallicity data is increased that evidence for the presence of correlated scatter about the MZR will solidify. Failure to find this trend observationally will indicate a serious point of tension in the IllustrisTNG feedback model.

7 CONCLUSIONS

In this paper we have analysed the metal distribution within the TNG100 simulation, part of the IllustrisTNG simulation suite, with a focus on the properties and evolution of the mass metallicity relation. The IllustrisTNG simulations contain a comprehensive feedback model that is aimed to regulate the stellar mass growth of galaxies, but this same feedback model has the impact of widely redistributing the metal budget into different gas phases (Fig. 1). While star formation – and therefore metal production – is associated with dense gas, the majority of gas-phase metals (~ 85 per cent at $z = 0$) in our simulated galaxies are found outside of the dense ISM (Fig. 2). Understanding the properties and evolution of the MZR therefore requires a combined understanding of the ISM metal retention efficiency and gas-mass evolution as a function of time and galaxy mass.

Our primary conclusions in this paper are as follows:

(i) The IllustrisTNG simulated MZR is in broad agreement with observations over the redshift range $0 < z < 2$ (Fig. 6). We find a gradual decline in the normalization of the MZR which is consistent with observations out to $z = 2$ and which we predict to continue out to $z = 6$ and beyond (Fig. 7).

(ii) However, there is a break in the simulated MZR for $z > 0$ associated with the minimum wind velocity used in the supernova wind model. Low-galaxy-mass MZR data is still somewhat sparse and so it is unclear if the break in the MZR is in tension with current observations. If so, it would imply that the minimum wind velocity which is needed to shape the galaxy stellar mass function in the IllustrisTNG model requires modification.

(iii) We showed that a majority of metals live outside of the ISM (Figs 1 and 2), and further that high-mass IllustrisTNG galaxies are less efficient at retaining their metals compared to their lower mass companions (Fig. 3). We calculated the redshift evolution of the metal retention efficiencies to identify the relative partitioning of metals between the ISM, CGM, and stars (Fig. 3).

(iv) We argued that the primary driver of the MZR normalization evolution is not an evolution of metal retention efficiencies, but rather the evolving galactic gas fractions. The ISM metal retention efficiency *increases* towards high redshift (Fig. 3) which should lead to an increase in the ISM metallicity. Instead, the decrease in the ISM metallicity towards high redshift is a result of high redshift galaxies having higher gas fractions (Figs 8 and 9). The higher gas fractions result in diluted/lower metallicities, even with high-ISM metal retention efficiencies.

(v) There is a clear correlation between the scatter in the MZR and galactic ISM gas-mass or SFR (Figs 9 and 10). The existence of correlated scatter about the MZR has been observationally postulated to constitute a ‘fundamental metallicity relation’. Our models recover a similar residual relationship between metallicity and ISM gas-mass as is found observationally (Fig. 10). While there remains observational uncertainty on the existence of the fundamental metallicity relation, our models clearly support the existence of such a relation.

(vi) Despite the existence of the fundamental metallicity relation in our simulated data, we find that galaxies do *not* move along the fundamental metallicity relation (Fig. 12). Instead, galaxies oscillate between periods of being enrichment and accretion dominated. The net trend is a very clear effective ‘restoring force’ that drives galaxies back to equilibrium ISM masses and metallicities (Fig. 13).

(vii) Many of the results reported and conclusions drawn in this paper with respect to the gas fraction dependence of the MZR evolution and presence of correlated residual scatter about the MZR are consistent with predictions from equilibrium models (Lilly et al. 2013; Forbes et al. 2014). In particular, our findings that changes in gas fraction play a dominant role in the redshift evolution of the MZR as well as in explaining the residual scatter about the MZR are qualitatively consistent with predictions from equilibrium models.

Complementary constraints on our models and the results presented in this paper can be obtained through closer examination of the metal budget in the CGM. While feedback has shaped the MZR in our simulations by expelling a significant fraction of the metal content from the star-forming ISM, much of this metal content remains in the CGM. More complete and comprehensive accounting of the metal budgets for non-ISM phases – including metals in the CGM, metals locked into stars, and metals depleted on to dust gains (McKinnon, Torrey & Vogelsberger 2016; McKinnon et al. 2017) – will likely prove important for constructing more fine-grained constraints on galactic feedback modelling.

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