Evolution of the atomic and molecular gas content of galaxies

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ABSTRACT
We study the evolution of atomic and molecular gas in galaxies in semi-analytic models of galaxy formation that include new modeling of the partitioning of cold gas in galactic discs into atomic, molecular, and ionised phases. We adopt two scenarios for the formation of molecules: one pressure-based and one metallicity-based. We find that both recipes successfully reproduce the gas fractions and gas-to-stellar mass ratios of H i and H 2 in local galaxies, as well as the H i and H 2 disc sizes up to z ≤ 2. We reach good agreement with the locally observed H i and H 2 mass function, although both recipes slightly overpredict the low-mass end of the H i mass function. Both of our models predict that the high-mass end of the H i mass function remains nearly constant at redshifts z < 2.0. The metallicity-based recipe yields a higher cosmic density of cold gas and much lower cosmic H 2 fraction over the entire redshift range probed than the pressure based recipe. These strong differences in H i mass function and cosmic density between the two recipes are driven by low mass galaxies (log (M ∗/M ⊙) ⩽ 7) residing in low mass halos (log (M vir/M ⊙) ⩽ 10). Both recipes predict that galaxy gas fractions remain high from z ∼ 6–3 and drop rapidly at lower redshift. The galaxy H 2 fractions show a similar trend, but drop even more rapidly. We provide predictions for the CO J = 1 − 0 luminosity of galaxies, which will be directly comparable with observations with sub-mm and radio instruments.

Key words: galaxies: formation - galaxies: evolution - galaxies: ISM - ISM: atoms - ISM: molecules

1 INTRODUCTION
Attaining an understanding of when, how, and at what rate stars form out of interstellar gas, and of the mechanisms that regulate this process, is of key importance in building up a complete picture of galaxy formation and evolution. Observations across a range of scales have shown that star-formation (SF) is tightly linked to galaxy gas content. Observations in our Milky Way have shown that star formation takes place in dense giant molecular clouds (GMC; e.g., Solomon et al. 1987; McKee & Ostriker 2007; Bolatto et al. 2008). Early observational work found a correlation between the surface density of the star formation rate (SFR) and the surface density of the total cold gas in galaxies (e.g. Schmidt 1959; Kennicutt 1998), while more recent work has emphasized that there is a strong correlation between the SFR density and the density of molecular hydrogen (H 2), while the correlation with atomic hydrogen (H i) is weak or absent (Wong & Blitz 2002; Bigiel et al. 2008, 2011; Schruba et al. 2011). This work has stimulated a desire to understand and track the H i and H 2 content of galaxies separately in theoretical models.

Observational studies of the H i and H 2 content of nearby galaxies have made great advances in recent years. The local H i mass function down to masses of log (M H i/M ⊙) = 7, and global H i density Ω H i, has been quantified by blind surveys such as ALFALFA (Giovanelli et al. 2005; Martin et al. 2010). The H i content and its relationship with other galaxy properties (such as stellar mass, stellar surface density, color, and concentration) have been quantified for a fairly large, homogeneously selected sample of nearby galaxies by GASS (Galex Arecibo SDSS survey: Catinella et al. 2010, 2012, 2013). The THINGS (The H i nearby galaxy survey: Walter et al. 2008) and LITTLE THINGS (Hunter et al. 2012) surveys mapped the atomic hydrogen density distribution in small samples of nearby galaxies.

The molecular hydrogen content of galaxies has most commonly been studied through emission from 12CO (from here on CO) as a tracer. The CO mass-function of nearby...
galaxies was presented by Keres, Yun & Young (2003), along
with an estimate of the $H_2$ mass-function resulting from
the application of a constant conversion factor between CO
luminosity and $H_2$ mass. An updated estimate of the $H_2$
mass function from the Keres, Yun & Young (2003) sample,
based on an empirical, and variable, CO-$H_2$ conversion
factor, was presented by Obreschkow & Rawlings (2009b). The
BIMA SONG (BIMA survey of nearby galaxies: Helfer et al.
2003), HERACLES (HERA CO-Line Extragalactic Survey:
Leroy et al. 2009) and COLD GASS (CO legacy database for
GASS: Saintonge et al. 2011) surveys mapped the CO-
emitting gas in galaxies of the THINGS and GASS surveys,
constraining the surface densities and gas-to-star ratios of
molecular gas.

Observations of atomic hydrogen in emission have up
until now been restricted to galaxies at redshifts of $z \lesssim
0.2$ (Verheijen et al. 2007; Catinella et al. 2008). Damped
Lyman-$\alpha$ absorbers (DLA) have provided estimates of the
global atomic hydrogen content of the Universe ($\Omega_{\text{gas}}$) at much
higher redshifts ($z < 4.5$; e.g., Rao, Turnshek & Nestor
2006; Prochaska & Wolfe 2009; Noterdaeme et al. 2012),
but the exact nature of these systems, and their connection
to galaxies detected in emission, is still unclear, making the
interpretation of these observations somewhat complicated
(Berry et al. 2013).

Direct observations of the molecular content of distant
galaxies through the CO line have recently become available
for small samples of objects, although these samples are usu-
ally biased towards the most gas-rich, actively star-forming
galaxies (e.g. Genzel et al. 2010; Tacconi et al. 2010; Riechers
et al. 2011; Bothwell et al. 2013; Tacconi et al. 2013). Al-
though results are still inconclusive because of the small and
potentially biased nature of the samples, and uncertainties
in the $H_2$-CO conversion factor, these studies suggest that
galaxies at high redshift may have been considerably more
rich in $H_2$ than nearby galaxies. Moreover, a tight relation-
ship between $H_2$ surface density and SFR density seems to
persist out to at least $z \sim 2$ (Genzel et al. 2010; Daddi et al.
2010).

The gas content of galaxies at high redshift has also
been estimated using more indirect methods, such as by us-
ing Far-Infrared (FIR) observations and an assumed rela-
tionship between dust and $H_2$ mass (Magdis et al. 2012), or
by using an empirical relationship between SFR density and
total gas or $H_2$ content along with SF tracers such as H-$\alpha$
or UV (Erb et al. 2006; Mannucci et al. 2009; Popping et al.
2012).

All of the above efforts have already led to extremely
valuable insights and constraints on galaxy formation mod-
els. However, our ability to measure HI and CO in emission,
in unbiased samples of galaxies out to high redshift, is
expected to undergo a revolution in the next decade, with new
and upcoming facilities such as the Atacama Large Millime-
ter Array (ALMA; Wootten & Thompson 2009) and the
Square Kilometer Array (SKA; Carilli & Rawlings 2004) and
its pathfinders the Karoo Array Telescope (MeerKAT;
Booth et al. 2009) and the Australian SKA Pathfinder
(ASKAP; Johnston et al. 2008) coming online.

The observations expected from these facilities present
a new and stringent challenge to theoretical models of galaxy
formation. Until recently, most cosmological models and
simulations of galaxy formation did not attempt to ‘par-
tition’ gas into different phases, and used a total-gas based
(HI +$H_2$) Kennicutt-Schmidt (KS) law to model star for-
mation. However, aided by the insights gained from studies
of the relationship between star formation and gas prop-
eries on $\sim kpc$ scales (e.g. Bigiel et al. 2008; Leroy et al.
2008) in external galaxies, theorists have also made consider-
able progress on developing physical models linking the effi-
ciency of star formation on GMC scales with that on galactic
scales. Several groups have implemented explicit mod-
eling of detailed chemistry and simplified radiative trans-
fer into galaxy-scale and cosmological numerical hydrody-
namic simulations, tracking the multi-phase gas content and
implementing $H_2$-based star formation prescriptions (e.g.
Pelupessy, Papadopoulos & van der Werf 2006; Robertson
& Kravtsov 2008; Gnedin & Kravtsov 2011; Christensen
et al. 2012; Kuhlen et al. 2012). Gnedin & Kravtsov (2011,
hereafter GK) presented fitting functions for the SFR in
their simulations as a function of total cold gas density ($\Sigma_{\text{HI}} + \Sigma_{\text{H}_2}$), gas phase metallicity, and the intensity of
the UV ionizing background. Krumholz, McKee & Tumlin-
sion (2009) presented analytic models for the formation of
$H_2$ as a function of total gas density and metallicity, sup-
ported by numerical simulations with simplified geometries
(Krumholz, McKee & Tumlinson 2008, 2009), emphasizing
the importance of metallicity as a controlling parameter in
$H_2$ formation. A somewhat different view is presented by Os-
triker, McKee & Leroy (2010), who propose that heating of
the Interstellar Medium (ISM) by the stellar UV background
plays a key role in regulating star formation. In their model,
the thermal pressure in the diffuse ISM, which is propor-
tional to the UV heating rate, adjusts until it balances the
midplane pressure set by the vertical gravitational potential.
This could provide an explanation for the strong empirical
correlation between $H_2$ fraction and disc midplane pressure
found by Blitz & Rosolowsky (2006).

These analytic models and fitting formulae can be im-
plemented within semi-analytic models of galaxy formation.
The modern semi-analytic approach applies simple, physi-
cally motivated recipes for physical processes that drive the
formation and evolution of galaxies within the framework of
a Λ cold dark matter (ΛCDM) cosmology. These models can
provide predictions of global galaxy properties (such as SFR,
size, stellar mass and luminosity, gas content, metal enrich-
ment) for large numbers of galaxies. Furthermore, they can
efficiently explore the parameter space associated with the
large number of "sub-grid" recipes that are used to model
processes such as star formation, stellar feedback, black hole
accretion and feedback from Active Galactic Nuclei (AGN).
Semi-analytic models have been successful in reproducing
many observed galaxy properties (e.g., Kauffmann, White
& Guiderdoni 1993; Cole et al. 1994; Kauffmann et al. 1999;
Somerville & Primack 1999; Cole et al. 2000; Somerville,
Primack & Faber 2001), in particular recent models that in-
clude ‘radio mode’ AGN feedback (e.g., Bower et al. 2006;
Croton et al. 2006; Kang, Jing & Silk 2006; Menci et al. 2006;
Monaco, Fontanot & Taffoni 2007; Somerville et al. 2008b),
although some puzzles remain. For example, SAMs from sev-
reral different groups do not correctly reproduce the observed
properties of low-mass galaxies ($\log (M_*/M_\odot) \sim 9 - 10.5$
Fontanot et al. 2009; Guo et al. 2010; Weimann et al. 2012).
These low-mass galaxies form too early in the models, and
are too passive at late times. On the other hand, SAMs

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have also had difficulty reproducing enough very rapidly star forming, extreme starbursts (Ultra-luminous Infrared Galaxies; ULIRGS) at high redshift (Somerville et al. 2012; Niemi et al. 2012, and references therein). However, numerical hydrodynamic simulations suffer from the same problems (Weinmann et al. 2012; Davé et al. 2010), and in fact produce very similar predictions to the SAMs, leading most theorists to conclude that it is likely to be limitations in our understanding of the sub-grid processes of star formation and stellar feedback, rather than inaccuracies of the semi-analytic approach, that are the root cause of the problems.

Several groups have now used semi-analytic models to make predictions for the multi-phase gas content of galaxies. Obreschkow et al. (2009a) applied an empirical pressure-based recipe based on the results of Blitz & Rosolowsky (2006, hereafter BR) in post-processing to compute the H\textsubscript{i} and H\textsubscript{2} content of galaxies in the Millennium simulations (De Lucia & Blaizot 2007). Power, Baugh & Lacey (2010) carried out a similar project based on post-processing, Fu et al. (2010, 2012) modeled the partitioning of gas into H\textsubscript{i} and H\textsubscript{2} in radial bins in each galaxy, using both the metallicity-dependent recipes of Krumholz, McKee & Tumlinson (2009, hereafter KMT) and the pressure-based recipe of BR, and self-consistently implemented a H\textsubscript{2}-based star formation recipe, within the established semi-analytic modeling framework of Guo et al. (2011). Lagos et al. (2011a,b) also estimated gas partitioning into an atomic and molecular component, and implemented a H\textsubscript{2}-based star formation recipe, within the GALEFORM semi-analytic model (Baugh et al. 2005; Bower et al. 2006). Somewhat simpler models in a similar spirit have also been presented by Dutton, van den Bosch & Dekel (2010) and Krumholz & Dekel (2012).

In this paper we explore how different models for H\textsubscript{2} formation affect the evolution of the atomic and molecular gas content of galaxies with time. We implement an empirical, pressure-based recipe (BR) and a recipe based on numerical hydrodynamic simulations, dependent on metallicity and the local UV radiation field (GK) into the Somerville et al. (2012) model, thus allowing a link to be made between the stellar and dust emission and the multi-phase gas content of galaxies. We anticipate that these predictions will be useful for planning upcoming observations of cold gas in galaxies at high redshift, and as these observations become available, this will provide insights into the physics that drives the formation of molecules in galaxies. Furthermore, we aim to give insight to what improvements need to be incorporated in cosmological galaxy evolution models to correctly model the gas content of galaxies. In Somerville, Popping & Trager (in prep.; SPT14) we implement a wider suit of star-formation and H\textsubscript{2} recipes including the KMT recipe. We will present predictions for the observable properties of the stellar (and dust) emission over a broad range of redshifts, and discuss the sensitivity of these properties to the adopted SF-recipes.

The structure of the paper is as follows. In Section 2 we briefly present the semi-analytic model and its ingredients, focussing on the new recipes for gas partitioning and star formation. In Section 3 we present our predictions for the scaling relations between stellar mass or surface density and H\textsubscript{i} and H\textsubscript{2} content, relationship between H\textsubscript{i} mass and radius, and H\textsubscript{i} and H\textsubscript{2} mass functions at \( z \sim 0 \). We further present predictions for the evolution in the SFR half-light radius vs. stellar mass, H\textsubscript{i} and H\textsubscript{2} mass functions, global mass density of H\textsubscript{i} and H\textsubscript{2}, and H\textsubscript{i} and H\textsubscript{2} fractions vs. stellar mass. We compare our predictions of H\textsubscript{2} fractions and mass functions with observational estimates of these quantities obtained by applying a CO-H\textsubscript{2} conversion factor to the observations; we also adopt an alternate approach in which we use our knowledge of the physical properties of our model galaxies to estimate the CO content, and compare directly with the CO observations. In Section 4 we discuss our findings and we summarize those in Section 5.

2 MODEL

This section describes the semi-analytic model used in this paper. The model is based on the models presented in Somerville & Primack (1999), Somerville et al. (2008b, and Somerville et al. 2012) and we refer the reader to those papers for details. In this section we provide a brief summary of the model framework and the ingredients relevant to this paper. Throughout this paper we adopt a flat ΛCDM cosmology with \( \Omega_0 = 0.28, \Omega_\Lambda = 0.72, h = H_0/(100\,\text{km}\,\text{s}^{-1}) = 0.70, \sigma_8 = 0.812 \) and a cosmic baryon fraction of \( f_b = 0.1658 \) (Komatsu et al. 2009). Unless stated otherwise we leave the free parameters associated with the galaxy-formation model fixed to the values given in Somerville et al. (2012).

2.1 Semi-analytic model framework

The merging histories of dark matter halos (merger trees) are constructed based on the Extended Press-Schechter formalism following the method described in Somerville & Kolatt (1999) and Somerville et al. (2008b). Each branch in the tree represents a merger event and is followed back in time to a minimum progenitor mass of \( M_{\text{min}} \), which we refer to as the mass resolution of our simulations.

Whenever dark matter halos merge, the central galaxy of the largest progenitor halo becomes the new central galaxy, whereas all the other galaxies become ‘satellites’. Satellite galaxies may eventually merge with the central galaxy due to dynamical friction. Merger timescale are estimated using a variant of the Chandrasekhar formula from Boylan-Kolchin, Ma & Quataert (2008). Tidal stripping and destruction of the satellites is included as described in Somerville et al. (2008b).

Before reionisation of the Universe, each halo contains a mass of hot gas equal to the universal baryon fraction times the virial mass of the halo. After reionisation, the collapse of gas into low-mass halos is suppressed by the photoionising background. We model the fraction of baryons that can collapse into halos of a given mass after reionisation using the fitting functions provided by Gaëtan (2000) and Kravtsov et al. (2004).

When a dark matter halo collapses or experiences a merger with a larger halo, the hot gas shock-heats to the virial temperature of the new halo. The radiating gas then gradually cools and collapses. To calculate the cooling rate of the hot gas we use the metallicity-dependent radiative cooling curves of Sutherland & Dopita (1993). The rate at which gas can cool is given by

\[ \dot{\rho}_{\text{cool}} = \frac{1}{2} \frac{m_{\text{hot}}}{\rho_{\text{vir}}} \frac{c_{\text{s}}}{\rho_{\text{vir}}} \frac{\rho_{\text{vir}}}{T_{\text{cool}}} \]  

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where $m_{\text{hot}}$ is the mass of the hot halo gas, $r_{\text{vir}}$ is the virial radius of the dark matter halo, and $r_{\text{cool}}$ is the radius within which all of the gas can cool in a time $t_{\text{cool}}$, which itself depends on density, metallicity and temperature. This cooling radius limited regime is associated with “hot flows”. In some cases the cooling radius can be larger than the virial radius. In this case the cooling rate is limited by the infall rate

$$\dot{m}_{\text{cool}} = \frac{1}{2} m_{\text{hot}} \frac{1}{t_{\text{cool}}}.$$  \hspace{1cm} (2)

This infall limited cooling regime is associated with “cold flows” (Birnboim & Dekel 2003; Kereš et al. 2005; Dekel & Birnboim 2006).

Although in reality satellite galaxies should continue to accrete some cold gas, we assume that cold gas is only accreted by the central galaxy of the halo. When the gas cools we assume it initially collapses to form a rotationally supported disc. The scale radius of the disc is computed based on the initial angular momentum of the gas and the halo profile, assuming that angular momentum is conserved and that the self-gravity of the collapsing baryons causes contraction of the matter in the inner part of the halo (Blumenthal et al. 1986; Flores et al. 1993; Mo, Mao & White 1998). Assuming that the halo initially has a density profile described by the Navarro-Frank-White (NFW; Navarro, Frenk & White 1996) form, the size of the gas disc of a galaxy is given by

$$r_{\text{gas}} = f_j \alpha \sqrt{f_c} f_{\text{c}}^{-1/2} f_h (\lambda, c, f_d),$$  \hspace{1cm} (3)

where $f_j \equiv (J_d/M_d)/(J_h/M_{hi})$ is the ratio of the specific angular momentum of the disc and the halo, $c$ is the NFW concentration of the halo, and $f_d$ is the disc mass to the halo mass ratio. The functions $f_c^{-1/2}$ correct for the difference in energy of the NFW profile relative to that of a singular isothermal profile, and $f_h$ accounts for the adiabatic contraction (see Mo, Mao & White 1998, for expressions governing $f_h$ and $f_j$ ). Somerville et al. (2008a) showed that this approach produced good agreement with the evolution of the size-stellar mass relation for disc-dominated galaxies from $z \sim 2$ to the present.

Stars are formed through two modes, a “normal” mode in isolated discs, and a merger-driven “starburst” mode. We discuss star formation in the “normal” mode in below Section 2.2. The efficiency and timescale of the “starburst” mode is set by the merger mass ratio and the gas fractions of the merger progenitors, based on the results of hydrodynamical simulations of binary galaxies (Robertson et al. 2006; Hopkins et al. 2009a).

When supernovae occur, they deposit some of their energy into the ISM, driving a large-scale outflow of cold gas from the galaxy. The mass outflow rate is given by

$$\dot{m}_{\text{out}} = \alpha SN \left( \frac{V_0}{V_c} \right) \dot{m}_*,$$  \hspace{1cm} (4)

where $V_c$ is the maximum circular velocity of the galaxy (here approximated by $V_{\text{max}}$ of the uncontracted dark matter halo), $\dot{m}_*$ is the star formation rate, and $\alpha_{SN}$ are free parameters ($V_0 = 200$ km/s is an arbitrary normalization constant). Some fraction of the ejected gas escapes from the potential of the dark matter halo, whereas some is deposited in the hot gas reservoir within the halo and can cool again. The fraction of gas ejected from the disc and halo versus ejected from the disc but retained in the halo is a function of the halo circular velocity, such that low-mass halos lose a larger fraction of gas (see Somerville et al. (2008b) for details). We choose $\alpha_{SN} = 1.5$ and $\alpha_{SN} = 2.2$ (similar to previous works) to obtain a good match with the observed $z \sim 0$ stellar mass function.

Each generation of stars produces heavy elements that can enhance the metal content of a galaxy. Here, chemical enrichment is modelled in a simple manner using the instantaneous recycling approximation. For each parcel of new stars $dM_*$, we also create a mass of metals $dM_G = y dM_*$, which we assume to be instantaneously mixed with the cold gas in the disc. We assume the yield $y$ to be constant, and treat it as a free parameter. When supernova driven winds eject gas from the disc, a corresponding proportion of metals is also removed and deposited either in the hot gas or outside the halo, following the same proportions as the ejected gas.

Mergers can remove angular momentum from the disc stars and build up a spheroid. The efficiency of disc destruction and build up of spheroids is a function of progenitor mass ratio and gas fractions, parameterised based on the simulations of binary galaxy systems (Hopkins et al. 2009a). These simulations indicate that more “major” and more gas-poor mergers are more efficient in removing angular momentum, destroying discs, and building spheroids. When implemented within the SAM, these recipes correctly predict the relative fractions of early vs. late type galaxies as a function of stellar mass (Hopkins et al. 2009b).

The model tracks the growth of supermassive black holes and the energy they release (Croton et al. 2006; Somerville et al. 2008b). Each top-level DM halo is seeded with a $\sim 100 M_\odot$ black hole, and these black holes are able to grow via two different accretion modes. The first accretion mode is fueled by cold gas that is driven into the nucleus of the galaxy by mergers. This mode is radiatively efficient, and the accretion rates are close to the Eddington limit. The accretion continues until the energy being deposited into the ISM in the central region of the galaxy is sufficient to significantly offset and halt accretion via a pressure-drive outflow. Because this accretion mode is associated with optically bright classical quasars and AGN, it is sometimes referred to as “bright mode” or “quasar mode” accretion. The second mode of black hole growth, the “radio mode”, is thought to be associated with powerful jets observed at radio frequencies. Hot halo gas is assumed to be accreted according to the Bondi-Hoyle approximation (Bondi 1952). We adjust the efficiency of “radio mode” heating to fit the observed number density of massive galaxies, and obtain $\kappa_{\text{radio}} = 3.8 \times 10^{-3}$. Accretion rates in this mode are significantly sub-Eddington ($10^{-4}$ to $10^{-3}$ times the Eddington rate), so that most of the BH’s mass is acquired during “bright mode” accretion. However, the radio jets are assumed to couple very efficiently with the hot gas, and provide a heating term that can partially or completely offset cooling during the “hot flow” mode.

### 2.2 Multi-phase Gas Partitioning and Star Formation Recipes

In this section we describe the new ingredients of our model that we use to calculate the fraction of ionised, atomic, and
molecular gas in each galaxy, and how we compute the SFR based on the molecular gas content.

At each time step we compute the scale radius of the cold gas disc using the angular momentum argument described in the previous subsection. We assume that the cold gas is distributed in an exponential disc with scale radius $r_{\text{gas}}$ and a central gas surface density of $m_{\text{cold}}/(2\pi r_{\text{gas}})^2$, where $m_{\text{cold}}$ is the mass of all cold gas in the disc. We assume that the stellar scale length is defined as $r_{\text{star}} = r_{\text{gas}}/\chi_{\text{gas}}$, with $\chi_{\text{gas}} = 1.7$ fixed to match stellar scale lengths at $z = 0$.

We divide the gas disc into radial annuli and compute the fraction of molecular gas in each annulus as described below. The integrated mass of H\textsc{i} and H\textsc{ii} in the disc at each time step is calculated using a fifth order Runge-Kutta integration scheme.

2.2.1 Ionised gas

We assume that the cold gas consists of an ionised, atomic and molecular component. The ionised component may be due to either an external background or by the radiation field from stars within the galaxy. We assume that some fraction of the cold gas in the galaxy, $f_{\text{ion, int}}$, is ionised by the stars in the galaxy. The external background field ionises a slab of gas on each side of the disc. Following Gnedin (2012), and assuming that all the gas with a surface density below some critical value $\Sigma_{\text{crit}}$ is ionised, we use

$$f_{\text{ion}} = \frac{\Sigma_{\text{HI}}}{\Sigma_0} \left[ 1 + \ln \left( \frac{\Sigma_0}{\Sigma_{\text{HI}}} \right) + 0.5 \left( \ln \left( \frac{\Sigma_0}{\Sigma_{\text{HI}}} \right) \right)^2 \right].$$

Where $\Sigma_0$ is the surface density at the critical value $\Sigma_{\text{HI}}$.

Throughout this paper we assume $f_{\text{ion, int}} = 0.2$ (as in the Milky Way) and $\Sigma_{\text{HI}} = 0.4 M_\odot pc^{-2}$, supported by the results of Gnedin (2012). Although observations do not support a sharp transition to ionized gas at this surface density, we found that our model reproduced the results of the hydro simulations well with this choice of parameters.

2.2.2 Molecular gas: pressure based partitioning

In this work we consider two approaches for calculating the molecular fraction of the cold neutral gas in a galaxy. The first is based on the empirical pressure-based recipe presented by Blitz & Rosolowsky (2006, BR). They found a power-law relation between the disc mid-plane pressure and the ratio between molecular and atomic hydrogen, i.e.,

$$R_{\text{H}_2} = \left(\frac{\Sigma_{\text{H}_2}}{\Sigma_{\text{HI}}} \right) = \left(\frac{P_m}{P_0}\right) ^\alpha$$

where $\Sigma_{\text{H}_2}$ and $\Sigma_{\text{HI}}$ are the H\textsc{ii} and H\textsc{I} surface density, $P_0$ and $\alpha_{\text{BR}}$ are free parameters that are obtained from a fit to the observational data, and $P_m$ is the mid-plane pressure acting on the galactic disc. We adopted $P_0/k_B = 4.23$ cm$^2$ K and $\alpha_{\text{BR}} = 0.8$ from Leroy et al. (2008). The hydrostatic pressure acting on the disc at a radius $r$ is estimated as (Elmegreen 1989, 1993; Fu et al. 2010)

$$P_m(r) = \frac{\pi}{2} G \Sigma_{\text{gas}}(r) [\Sigma_{\text{gas}}(r) + f_\text{gas}(r) \Sigma_\star(r)]$$

where $G$ is the gravitational constant, $f_\text{gas}(r)$ is the ratio between $\Sigma_{\text{gas}}(r)$ and $\sigma_\star(\mathbf{r})$, the gas and stellar vertical velocity dispersion, the stellar disc density profile $\Sigma_\star(\mathbf{r})$ is modeled as an exponential with scale radius $r_{\text{star}}$.

and central density $\Sigma_{\star, 0} \equiv m_\odot/(2\pi r_{\text{star}}^2)$. Following Fu et al. (2010), we adopt $f_\text{gas}(r) = 0.1 \sqrt{\Sigma_\star(\mathbf{r})/\Sigma_{\star, 0}}$, based on empirical scalings for nearby disc galaxies. The fraction of non-ionized gas in a molecular state at each radial annulus can be calculated as $f_{\text{H}_2} = R_{\text{H}_2}/(1 + R_{\text{H}_2})$.

2.2.3 Molecular gas: metallicity based partitioning

The second approach for computing molecular gas fractions in galaxies is based on the simulation by Gnedin & Kravtsov (2011, GK), who performed high-resolution “zoom-in” cosmological simulations with the Adaptive Refinement Tree (ART) code of Kravtsov (1999), including gravity, hydrodynamics, non-equilibrium chemistry, and 3D on the fly radiative transfer. Based on their simulations, the authors find a fitting function for the $\text{H}_2$ fraction which effectively parameterizes $f_{\text{H}_2}$ as a function of dust-to-gas ratio relative to the Milky Way, $D_{\text{MW}}$, the UV ionizing background relative to the Milky Way, $U_{\text{MW}}$, and the neutral gas surface density $\Sigma_{\text{HI+H}_2}$.

The fraction of molecular hydrogen at each radial annulus is given by

$$f_{\text{H}_2}(r) = \left[ 1 + \frac{\Sigma}{\Sigma_{\text{HI+H}_2}(r)} \right]^{-2}$$

where

$$\Sigma = 20 M_\odot pc^{-2} A_{\text{f}}^{4/7} \frac{1}{D_{\text{MW}} \left( 1 + U_{\text{MW}} D_{\text{MW}} \right)^{1/2}}$$

$$A = \ln(1 + g D_{\text{MW}}^{3/7} (U_{\text{MW}}/15)^{4/7})$$

$$g = 1 + \alpha s + s^2$$

$$s = 0.04$$

$$\alpha = 5 \frac{U_{\text{MW}}/2}{1 + (U_{\text{MW}}/2)^2}$$

$D_{\star} = 1.5 \times 10^{-3} \ln(1 + (3U_{\text{MW}})^{1.7})$

We take the dust-to-gas ratio to be proportional to the metallicity in solar units $D_{\text{MW}} = Z/Z_\odot$. The local UV background relative to the MW is set by relating the SFR of the galaxy in the previous time step to the MW SFR as $U_{\text{MW}} = \frac{SFR_{\text{MW}}}{\pi R_{\text{MW}}}$. We choose $SFR_{\text{MW}} = 1.0 M_\odot$ yr$^{-1}$ (Murray & Rahman 2010; Robitaille & Whitney 2010).

The GK fitting functions are intended to characterize the formation of molecular hydrogen on dust grains, the dominant mechanism for forming H\textsc{ii} once gas is enriched to more than a few hundredths of Solar metallicity. Other channels for the formation of H\textsc{ii} in primordial gas must be responsible for producing the molecular hydrogen out of which the first stars were formed. Hydrodynamic simulations containing detailed chemical networks and analytic calculations have shown that H\textsc{ii} can form through other channels in dark matter halos above a critical mass $M_{\text{crit}} \sim 10^9 M_\odot$ (e.g., Nakamura & Umemura 2001; Glover 2013). This gas can then form “Pop III” stars which can enrich the surrounding ISM to $Z_{\text{HII}} \sim 10^{-3} Z_\odot$ (Schneider et al. 2002; Greif et al. 2010; Wise et al. 2012). These processes take place in halos much smaller than our resolution limit. We represent them by setting a “floor” to the molecular hydrogen fraction in our halos, $f_{\text{H}_2, \text{floor}}$. In addition, we “pre-enrich” the initial hot gas in halos, and the gas accreted onto halos due to
with $\Sigma_{*}$ that the star-formation rate surface density can be directly obtained from the profiles presented in Leroy et al. (2008). The grey triangles and dots, blue squares, and red circles are literature values from Leroy et al. (2008), Saintonge et al. (2011), Catinella et al. (2013), and Boselli et al. (2014), respectively.

The star-formation rate surface density can be directly obtained from the profiles presented in Leroy et al. (2008). The grey triangles and dots, blue squares, and red circles are literature values from Leroy et al. (2008), Saintonge et al. (2011), Catinella et al. (2013), and Boselli et al. (2014), respectively.

2.2.4 Molecular based star formation

Star formation is modeled following empirical relationships from recent observations. Bigiel et al. (2008) suggest, based on observations of spiral galaxies from the THINGS survey, that the star-formation rate surface density can be directly related to the surface density of molecular gas, i.e.

$$\Sigma_{\text{SFR}} = A_{\text{SF}} \Sigma_{\text{H}_2} N$$

with $N \approx 1$. Observations of higher density environments suggest that above some critical $\text{H}_2$ surface density, the slope of the relation described in equation 9 steepens. We therefore adopt a two-part scaling law given by

$$\Sigma_{\text{SFR}} = A_{\text{SF}} \left( \frac{\Sigma_{\text{H}_2}}{10M_\odot \text{pc}^{-2}} \right) \left( 1 + \frac{\Sigma_{\text{H}_2}}{\Sigma_{\text{H}_2,\text{crit}}} \right)^{N_{\text{SF}}}$$

We adopt the “two-slope” star formation recipe in all of the models presented in this work. In addition, we adopt $A_{\text{SF}} = 5.98 \times 10^{-3} M_\odot \text{yr}^{-1} \text{kpc}^{-2}$, $\Sigma_{\text{H}_2,\text{crit}} = 70 M_\odot \text{pc}^{-2}$, and $N_{\text{SF}} = 1.0$. The value of $A_{\text{SF}}$ is taken from the observations of Bigiel et al. (2008), corrected to our system in which Helium is not included in the gas masses and densities. The values for $\Sigma_{\text{H}_2,\text{crit}}$ and $N_{\text{SF}} = 1.0$ are motivated by

Figure 2. The ratio of ionised hydrogen to stellar mass in disc-dominated galaxies ($M_{\text{total}}/M_{\text{H}_2} \leq 0.4$) as a function of stellar mass for the pressure- (solid orange) and metallicity-based (green dashed) $\text{H}_2$ formation recipes. Thick lines show the mean, and dotted lines mark the 2$\sigma$ deviation.
In this section we show our predictions for the evolution of the H\textsubscript{i} and H\textsubscript{2} content of galaxies over a range of redshifts from \( z = 0.0 \) to \( z = 6.0 \). The simulations were run on a grid of halos with virial masses ranging from \( 5 \times 10^8 \text{M}_\odot \) to \( 5 \times 10^{14} \text{M}_\odot \) with a mass resolution of \( 5 \times 10^6 \text{M}_\odot \). We first perform a comparison of our model predictions with observations of local galaxy properties, in order to validate our models. All presented gas masses are pure hydrogen masses and do not include a correction for Helium.

### 3 RESULTS

In this section we show our predictions for the evolution of the H\textsubscript{i} and H\textsubscript{2} content of galaxies over a range of redshifts from \( z = 0.0 \) to \( z = 6.0 \). The simulations were run on a grid of halos with virial masses ranging from \( 5 \times 10^8 \text{M}_\odot \) to \( 5 \times 10^{14} \text{M}_\odot \) with a mass resolution of \( 5 \times 10^6 \text{M}_\odot \). We first perform a comparison of our model predictions with observations of local galaxy properties, in order to validate our models. All presented gas masses are pure hydrogen masses and do not include a correction for Helium.

#### 3.1 Local galaxy properties

In Figure 1 we present the ratios of H\textsubscript{i} and H\textsubscript{2} relative to stellar mass, and the ratio of H\textsubscript{2} to H\textsubscript{i}, as functions of stellar mass and stellar surface density in disc-dominated galaxies \( (M_{\text{bulge}}/M_{\text{stellar}} \lesssim 0.4) \). We compare our results to a compilation of observations presented in Leroy et al. (2008), Saintonge et al. (2011), and Catinella et al. (2013) based on the THINGS+HERACLES and GASS+COLDGASS surveys and in Boselli et al. (2014) based on the Herschel reference survey.

Both the pressure-based and metallicity-based recipes show very good agreement with the observed trends between stellar mass or stellar surface density and H\textsubscript{i} and H\textsubscript{2} fractions. The fraction of H\textsubscript{i} relative to stars decreases with increasing stellar mass and surface density, whereas the fraction of H\textsubscript{2} relative to stars remains roughly constant. Consequently, the fraction of cold gas in the form of H\textsubscript{2} increases with stellar mass and surface density. The H\textsubscript{2}-to-H\textsubscript{i} ratio as a function of stellar mass is on average slightly too high in our models, although still within the scatter of the observations (particularly at low stellar masses). Here we focus on the gas fractions of disc-dominated galaxies. A similar exercise for a “blind” survey of galaxies would yield lower H\textsubscript{i}-to-stellar mass, H\textsubscript{2}-to-stellar mass, and H\textsubscript{2}-to-H\textsubscript{i} mass ratios. Spheroidal objects have much lower relative gas content than disc-dominated galaxies and most of the cold gas is atomic.

We present the ratio of ionised hydrogen to galaxy stellar mass as a function of stellar mass in Figure 2. We find a monotonic decrease in the ratio between ionised hydrogen and stellar mass, without any significant difference between...
of the gas, one of the key parameters in calculating the H\textsubscript{ scorned} size of the galaxy disc, as this sets the surface density of the gas. It is therefore of great importance to correctly predict the sizes of the gas disc in galaxies. Figure 3 shows the contribution to the mass function by galaxies with a lower cutoff in stellar mass. The bottom row shows the contribution from galaxies hosted by a halo with a lower cutoff in virial mass. Grey circles and diamonds are the estimated observed $z = 0$ H\textsubscript{2} mass functions from Keres, Yun & Young (2003), grey squares are the observational estimates presented by Obreschkow & Rawlings (2009b) (see text).

The good agreement between model and data is independent of the H\textsubscript{2} formation prescription. We have shown that our models match the observed H\textsubscript{2} fractions for nearby galaxies (Fig. 1), and Somerville et al. (2008a) has shown previously that the models also reproduce the size-stellar mass relation for disc-dominated galaxies from $z \sim 2$ to the present. Although this does not necessarily guarantee a match between the H\textsubscript{2} disc size and gas content of a galaxy, the agreement is an encouraging sanity check.

Figure 4 shows our predictions for the H\textsubscript{2} mass-functions at $z = 0.0$. Both star formation recipes show decent agreement with the observed H\textsubscript{2} mass functions at H\textsubscript{2} masses of log ($M_{\text{HI}}/M_\odot$) $\sim 10$ and higher. The pressure-based recipe slightly underpredicts the observed H\textsubscript{2} mass function in the mass range log ($M_{\text{HI}}/M_\odot$) $\sim 9$–10, and slightly overpredicts the observations at lower H\textsubscript{2} masses. The metallicity-based...
Evolution of atomic and molecular gas in galaxies

Figure 6. The SFR half-light radii of galaxies as a function of their stellar mass for different redshift bins, for the pressure-based (orange solid) and metallicity-based (green dashed) models. Thick lines show the mean of the distribution, and dotted lines mark the 2σ deviation. Grey circles are observations from Leroy et al. (2008, at z = 0.0), Förster Schreiber et al. (2009, Hα half light radii), Genzel et al. (2010) and Tacconi et al. (2013).

Figure 7. Predicted redshift evolution of the H I mass function, assuming a pressure- (left) and metallicity-based (right) H2 recipe. Grey circles and squares show the observed z = 0 mass functions from Zwaan et al. (2005) and Martin et al. (2010), respectively.

recipe overpredicts the observed number of galaxies below log (M_{HI}/M_☉) ~ 8.5.

Figure 4 shows that the galaxies responsible for the excess of low-HI mass objects are low-mass galaxies (log (M_☉/M_☉) ≤ 7) residing in low mass halos (log (M_{vir}/M_☉) ≤ 10). This underlines the importance of sufficiently high mass resolution in simulations that attempt to predict the properties of galaxies observed in HI.

The predicted H2 mass function at z = 0.0 is presented in Figure 5, and compared with two observational estimates. Both estimates are based on the CO survey of Keres, Yun & Young (2003). The estimated H2 mass func-

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ties. Based on recent observations and theoretical work, a significantly overproduce galaxies with large H. Oberschekow & Rawlings (2009b) estimated a variable H₂-CO conversion factor based on the galaxy properties. Based on recent observations and theoretical work, a variable conversion factor that depends on galaxy properties (such as metallicity) is probably more reasonable (we discuss this further below). The predictions of both recipes are very similar, and we obtain good agreement with the observational estimates of Keres, Yun & Young (2003), but significantly overproduce galaxies with large H₂ masses relative to the Oberschekow & Rawlings (2009b) results. It is possible that a process not included in our model, such as AGN feedback, could destroy or expel H₂ in massive galaxies (Santonge et al. 2012) and possibly lower the number of H₂ massive galaxies.

3.2 Evolution of gas in galaxies

In this section we present our predictions for the evolution of the gas content in galaxies and make predictions for upcoming surveys of gas at high redshifts.

3.2.1 Galaxy sizes

Figure 6 shows the SFR half-light radius of our modelled galaxies as a function of their stellar mass (i.e., the radius that encompasses half of the total SFR of the galaxy). We compare these results with radii presented in the literature for high-redshift galaxies (Förster Schreiber et al. 2006; Genzel et al. 2010; Tacconi et al. 2013) and, where possible, the CO half-light radius of the discs of the THINGS galaxies, which we computed from the radial profiles presented in (Leroy et al. 2008, assuming a fixed conversion between the H₂ and CO radial profiles). Our results are in excellent agreement with the observations at high-redshift and in the local Universe, indicating that in spite of the simplicity of our model for computing disc sizes and surface density profiles, we appear to be able to correctly model the sizes and the location of star formation and the evolution of these quantities since z = 2. For a fixed stellar mass, the SFR half-light radius increases with decreasing redshift. Consequently, the molecular gas is more compact in high redshift galaxies. This behavior is driven by the overall growth of galaxy discs with time, as they accrete gas with higher angular momentum.

3.2.2 H I mass function

Figure 7 shows the predicted H I mass function at redshifts between z = 0 and z = 6. We overplot observations from Zwaan et al. (2005) and Martin et al. (2010) at z = 0. For H I masses (log (M_HI/M☉) ≥ 8), the figure shows a clear monotonic increase in the number of galaxies at a given H I mass from z = 6 to z = 2.0. There is very weak evolution at z < 2, and almost none at all from z ~ 1–0. The weak evolution in the number of low HI mass galaxies shows that in our current model framework, the excess of these objects is already present at redshifts ~ 2. We find little difference in the predicted evolution of the HI mass function between the metallicity- and pressure-based recipes.

Although little evolution is seen in the HI mass function since z ~ 2, this of course does not mean that galaxies are static, or that HI is not being created or destroyed. It rather means that there is a kind of self-regulated equilibrium that arises naturally in these models.

3.2.3 H₂ mass function

In Figure 8 we show the predicted H₂ mass function at redshifts between z = 0 and z = 6. The left panel contains mass functions obtained using the metallicity-based

![Figure 8](image-url)
Evolution of atomic and molecular gas in galaxies

Both H$_2$ recipes predict a gentle evolution in the H$_2$ mass function at all H$_2$ masses. In both recipes, the number of galaxies with large H$_2$ masses increases from $z \sim 6$–2, then declines slightly to $z = 0$. At lower masses, log ($M_{H2}/M_\odot$) $\lesssim$ 9, both models predict a slight increase in the number of low-H$_2$ mass galaxies from $z \sim 6$–4, then a more or less monotonic decline from $z \sim 4$ to $z \sim 0$.

In both recipes, it is more difficult to form H$_2$ in low-surface density gas. In our models, low-mass halos host galaxies with a larger fraction of their gas at low surface density (this is in accord with observational size-mass scaling relations), and therefore low-mass galaxies are less efficient at forming H$_2$, as we saw in Figure 1. In the BR model, we would say this is because their disc midplane pressure is lower due to their smaller gravitational potential wells. In the GK model, we would say it is due to the lower availability of dust grains on which H$_2$ can form. Thus the build-up of large H$_2$-mass galaxies from $z \sim 6$–2 reflects the growth of structure and the formation of massive dark matter halos, while the decrease in the number of low-H$_2$ mass galaxies from $z \sim 4$ to $z \sim 0$ reflects the growth of galaxy discs resulting in lower cold gas surface densities, combined with low potential wells and/or low availability of dust grains.

3.2.4 Evolution in galaxy gas-fractions

In the following figures we present the gas fraction and relative H$_2$ content of galaxies as a function of their stellar mass for different redshifts ($0 < z < 6$). In each case, we plot the conditional probability $P(f_{\text{gas}}|m_{\text{star}})$, and the reader should keep in mind that the most massive galaxies will be extremely rare at high redshift, and probably would not be included in any observed samples.

Figure 9 shows the cold gas fraction of the modeled galaxies as a function of stellar mass, divided into redshift bins. We also included the indirectly derived gas fraction from Popping et al. (2012). They calculated cold gas and H$_2$ masses in galaxies from the COSMOS survey by inver-
metallicity-based recipe predicting slightly larger gas fractions. Only in low mass galaxies (log(\(M_\ast\)) ⩽ 9) do the two applied recipes give different predictions, with the metallicity-based recipe predicting slightly larger gas fractions. Including a recipe to calculate the H\(_2\) fraction of cold gas allowed Popping et al. to indirectly estimate both the molecular and the atomic hydrogen masses of these galaxies.

Our models predict that gas fractions decrease only mildly from \(z \sim 6-3\). At lower redshifts the gas fractions decrease rapidly, such that galaxies with large stellar masses run out of gas first. This evolution is similar for both H\(_2\) recipes. Only in low mass galaxies (log(\(M_\ast\)/\(M_\odot\)) ⩽ 9) do the two applied recipes give different predictions, with the metallicity-based recipe predicting slightly larger gas fractions. We find that our model predictions are in good agreement with the indirect estimates of Popping et al. (2012) for \(z \leq 1.0\). In the mass range log(\(M_\ast\)/\(M_\odot\)) > 10. At higher redshifts we find good agreement for objects with log(\(M_\ast\)/\(M_\odot\)) > 10.5. We overpredict the indirect estimates from the literature at lower stellar mass, however, we did not take the selection criteria applied by Popping et al. into account here.

Figure 10 shows \(f_{\text{H}_2} \equiv \frac{M_{\text{H}_2}}{M_{\ast}+M_{\text{H}_2}}\) as a function of stellar mass at different redshifts. We included a compilation of observations presented in Narayanan, Bothwell & Davé (2012, taken from Genzel et al. (2010); Daddi et al. (2010); Tacconi et al. (2010); Casey et al. (2011); Bothwell et al. (2013)) and in Tacconi et al. (2013). Besides the H\(_2\) masses quoted in the original literature, Narayanan, Bothwell & Davé (2012) uses a novel approach to calculate the conversion between CO observation and H\(_2\) masses and their resulting gas fractions (see section 3.3 for a detailed description). We included the original values for \(f_{\text{H}_2}\) as well as the recalibrated values. Similar to the previous figure, there is no significant difference between the two studied recipes. The evolution in \(f_{\text{H}_2}\), however, is much stronger. At \(z = 0.0\) we find \(f_{\text{H}_2} \sim 0.1\) at all probed stellar masses, whereas at \(z = 6.0\) we find values of \(f_{\text{H}_2} \sim 0.8\) over a large range of stellar masses. There is large scatter in \(f_{\text{H}_2}\) at redshifts \(z = 3.0 – 0.5\) over all probed stellar masses. This scatter is indicative of a transi-

Figure 10. Molecular fraction \(\frac{M_{\text{H}_2}}{M_{\text{H}_2}+M_{\ast}}\) as a function of stellar mass in disc-dominated galaxies for different redshift bins for the pressure-based H\(_2\) prescription (left column) and the metallicity-based prescription (right column). Blue shading shows the log of the conditional probability distribution function \(P(M_{\text{H}_2}/M_\ast)\), whereas the red solid line shows the median fit. Grey circles and red squares are estimates taken from Narayanan, Bothwell & Davé (2012) using the traditional and newly calculated value for the CO-to-H\(_2\) conversion, respectively. Green diamonds are observations from Tacconi et al. (2013). The black dashed and dotted lines show the mean and two sigma confidence region of the gas fractions presented in Popping et al. (2012).
Figure 11. Molecular fraction \( \frac{M_{\text{H}_2}}{M_*} \) as a function of stellar mass for different redshift bins, assuming a metallicity-based star formation law. We applied the selection criteria for Popping et al. (2012, COSMOS, \( I_{AB} < 24 \); left column) and CANDELS (\( H_{AB} < 25 \); right column). Blue shading shows the log of the conditional probability distribution function \( P(\frac{M_{\text{H}_2}}{M_*} | M_*) \), whereas the red solid line shows the median fit. The dashed and dotted lines represent the mean and two sigma confidence region of the gas fractions presented in Popping et al. (2012). Grey circles, red squares, and green diamonds are as in Figure 10.

This strong evolutionary trend, compared to the trends seen for the total cold gas fraction, indicates that the amount of \( \text{H}_2 \) decreases not only due to the availability of less cold gas, but that the \( \text{H}_2 \) fraction itself also drops (Popping et al. 2012). The rate at which this happens is independent of adopted recipe in our models. We find good agreement with the observations and their re-analysis by Narayanan, Bothwell & Davé (2012). Our model does not strongly favor either choice for the CO-\( \text{H}_2 \) conversion factor. Similar to the total cold gas fractions, we find that our model predicts a lower relative \( \text{H}_2 \) content of galaxies than the indirect estimates by Popping et al. (2012) suggest (especially at stellar masses \( \log (M_* / M_{\odot}) < 10.5 \)). We again emphasize that so far, we did not take the selection bias inherent to the observations that went into Popping et al. (2012) analysis into account. We will now discuss how selection criteria affect our results.

Current samples of high-redshift galaxies are highly sensitive to their selection criteria and direct observation of the molecular content of the galaxies are usually biased towards the most gas rich galaxies. To study how this bias might affect the comparison of our model predictions with observations in the literature, we apply the selection criteria from the relevant surveys to our model galaxies assuming a metallicity-based \( \text{H}_2 \) recipe and show the results in Figure 11. We compare our results to the gas fraction estimates for galaxies taken from the COSMOS sample with \( I_{AB} < 24 \) (Popping et al. 2012). We also show predictions for a sample with \( H_{AB} < 25 \) mag, representative of galaxies in the CANDELS survey (Grogin et al. 2011; Koekemoer et al. 2011) for which reliable measurements of galaxy size are expected to be able to be obtained.

When we account for the selection effects, we find good agreement with the indirect \( \text{H}_2 \) fraction estimates from the COSMOS sample. At \( z > 1.5 \) our model predicts slightly lower gas fractions than those suggested by the indirect estimates. The rough agreement is a very encouraging result for our model, but also emphasizes how important it is to properly take selection criteria into account when comparing models to observed galaxy samples. Our results also suggest
The cosmic comoving density, in units of the critical density, of cold gas (H\textsubscript{i} + H\textsubscript{2} + H\textsubscript{ii}; top panel), H\textsubscript{i} (middle) and H\textsubscript{2} (bottom) as a function of redshift. The solid orange line shows the pressure-based and the green dashed line shows the metallicity-based H\textsubscript{2} recipes. Observations of P\textregistered{}eroux et al. (2005); Rao, Turnshek & Nestor (2006); Guimar\~{a}es et al. (2009); Prochaska & Wolfe (2009) are overplotted in light gray. Dark gray observations are by Zafar et al. (2013) and observations from Noterdaeme et al. (2012) and local galaxies (Keres, Yun & Young 2003; Zwaan et al. 2005; Martin et al. 2010; Obreschcow & Rawlings 2009b; Braun 2012) are overplotted in black.

Figure 12. The cosmic comoving density, in units of the critical density, of cold gas (H\textsubscript{i} + H\textsubscript{2} + H\textsubscript{ii}; top panel), H\textsubscript{i} (middle) and H\textsubscript{2} (bottom) as a function of redshift. The solid orange line shows the pressure-based and the green dashed line shows the metallicity-based H\textsubscript{2} recipes. Observations of P\textregistered{}eroux et al. (2005); Rao, Turnshek & Nestor (2006); Guimar\~{a}es et al. (2009); Prochaska & Wolfe (2009) are overplotted in light gray. Dark gray observations are by Zafar et al. (2013) and observations from Noterdaeme et al. (2012) and local galaxies (Keres, Yun & Young 2003; Zwaan et al. 2005; Martin et al. 2010; Obreschcow & Rawlings 2009b; Braun 2012) are overplotted in black.

that repeating the analysis on the deeper, H-band selected CANDELS sample will greatly expand the range of stellar mass and gas fraction that can be probed by the indirect method at \( z > 1.5 \). We intend to repeat the Popping et al. (2012) analysis on the CANDELS sample in the near future. These results will provide an interesting complement to direct measures of high redshift gas fractions that will become available from ALMA.

3.2.5 Gas density evolution of the Universe

Figure 12 shows the predicted global H\textsubscript{i}, H\textsubscript{2}, and total cold gas density (including ionised hydrogen) of the Universe as a function of time (in units of the critical density). We compare our results to local H\textsubscript{i} and H\textsubscript{2} densities (Keres, Yun & Young 2003; Zwaan et al. 2005; Obreschcow & Rawlings 2009b; Martin et al. 2010; Braun 2012) and high-z estimates of the H\textsubscript{i} density obtained from Damped Lyman-\( \alpha \) (DLA) absorption systems (e.g., P\textregistered{}eroux et al. 2005; Rao, Turnshek & Nestor 2006; Guimar\~{a}es et al. 2009; Prochaska & Wolfe 2009; Noterdaeme et al. 2012; Zafar et al. 2013).

We see that the two H\textsubscript{2} formation recipes differ significantly in terms of both the total cold gas content of the Universe and the ratio between H\textsubscript{i} and H\textsubscript{2}. The metallicity-based recipe predicts more cold gas overall at all redshifts, and also more H\textsubscript{i}. The pressure-based recipe produces more H\textsubscript{2} overall, in spite of the lower amount of total cold gas. Both models underpredict \( \Omega_{\text{HI}} \) inferred from DLAS at \( z \geq 3 \).
the pressure-based model more dramatically. On the other hand, predictions by the metallicity-based model is in decent agreement with DLA observations at $z < 2.5$. Overall the metallicity-based recipe is better in reproducing the observed values for $\Omega_{\text{HI}}$ and $\Omega_{\text{H}_2}$.

The two $\text{H}_2$ formation recipes show a very different evolution in the global ratio of $\text{HI}$ to $\text{H}_2$ with redshift (see Figure 13). The pressure-based recipe predicts a monotonic increase in $\Omega_{\text{H}_2}/\Omega_{\text{HI}}$ and $\Omega_{\text{H}_2}/M_{\text{HI}}$ with increasing redshift. The metallicity-based recipe predicts a very mild increase with increasing redshift up to $z > 3.0$, then a flattening at higher redshifts. Especially worthwhile to note is that $\Omega_{\text{H}_2}$ never exceeds $\Omega_{\text{HI}}$ for the metallicity-based recipe, whereas it does by up to a factor of three for the pressure-based recipe. We will give a detailed discussion about the origin of these differences, and how they can help to constrain the physics driving the partitioning of hydrogen into atomic and molecular hydrogen, in Section 4.

As a comparison we also show predictions from Obreschkow & Rawlings (2009a) and Lagos et al. (2011a) in Figure 13. Both authors use a pressure-based recipe similar to ours. Although the predictions differ in detail — unsurprising as many other aspects of the models differ — we find that our predictions for the pressure-based recipe are in qualitative agreement with other predictions from the literature, indicating a strong decline in $\Omega_{\text{H}_2}/\Omega_{\text{HI}}$ with time. The slope of the decline differs significantly between the compared models. Only at $z > 4.0$ do the Lagos et al. models predict an increase in $\Omega_{\text{H}_2}/\Omega_{\text{HI}}$ with time. The authors claim this is due to a Monte-Carlo extension of the merger trees to very low mass halos dominated by $\text{HI}$, although our halo mass resolution is actually higher than theirs, so this seems unlikely to account for the difference with our results. Our predicted evolution in $\Omega_{\text{H}_2}/\Omega_{\text{HI}}$ for the metallicity-based $\text{H}_2$ recipe is much flatter compared with the predictions from pressure-based recipes.

3.3 Predictions in Observation Space

Our model gives predictions for the $\text{H}_2$ mass and surface density of galaxies, but these are difficult to observe directly. Observations typically use the CO luminosity as a tracer for the $\text{H}_2$ content of a galaxy, assuming a CO-to-$\text{H}_2$ conversion factor. A proper prediction of the CO luminosity of galaxies requires the inclusion of detailed chemistry and radiative transfer calculations (Lagos et al. 2012; Popping et al. 2013). In the present work we use a CO-to-$\text{H}_2$ conversion relation to convert our predicted $\text{H}_2$ masses to more directly observable CO luminosities. The advantage of working in “Observation Space” is that the CO-to-$\text{H}_2$ conversion factor is thought to depend on galaxy properties such as internal density and metallicity, which are predicted by our models. Thus instead of attempting to convert CO luminosities to $\text{H}_2$ masses for the observations, we can instead make use of our knowledge of our model galaxy properties to make a more physically motivated galaxy-by-galaxy conversion from $\text{H}_2$ to CO.

Recently, Narayanan et al. (2012) and Feldmann, Gnedin & Kravtsov (2012) coupled sub-grid models of the ISM with cosmological simulations of galaxy formation to calculate the CO-$\text{H}_2$ conversion factor for galaxies with different properties. Using a coupling of an $\text{H}_2$-formation model and radiative-transfer calculations to simulated isolated and starburst galaxies, Narayanan et al. (2012) found that the average CO-$\text{H}_2$ conversion factor in galaxies can be represented by

$$X_{\text{CO}} = \frac{1.3 \times 10^{21}}{Z^* \times \Sigma_{\text{H}_2}}$$

with $X$ in units of $\text{cm}^{-2} (\text{K km s}^{-1})^{-1}$, $\Sigma_{\text{H}_2}$ is the $\text{H}_2$ surface density in units of $M_\odot \text{pc}^{-2}$ and $Z^*$ is the gas metallicity in solar units.

Feldmann, Gnedin & Kravtsov (2012) use a coupling of sub-grid ISM models by Glover & Mac Low (2011) with cosmological simulations by Gnedin & Kravtsov (2011). They find that, when averaged on kiloparsec scales, the CO-$\text{H}_2$ conversion factor is weakly dependent on column density and radiation field and can be described as a function of metallicity:

$$\log (X_{\text{CO}}) = a_1 \log (Z^*) + a_2$$

with $a_1 = -0.66$ and $a_2 = 20.5$ (see the Feldmann, Gnedin & Kravtsov 2010 results averaged to 4 kpc).

We estimate the CO luminosities of our model galaxies by applying three different assumptions for the CO-$\text{H}_2$ conversion factor; a fixed conversion of $X_{\text{CO}} = 2 \times 10^{20} \text{cm}^{-2} (\text{K km s}^{-1})^{-1}$, the approach presented by Narayanan et al. (2012) and that of Feldmann, Gnedin & Kravtsov (2012). Note that all CO luminosities presented here correspond to the CO J=1-0 transition.

Figure 14 shows the CO luminosity of our model galaxies as a function of stellar mass at $z = 0.0$ for the three CO-$\text{H}_2$ conversion methods. Overplotted are CO luminosities observed by Leroy et al. (2008) and Saintonge et al. (2011). These CO luminosities have been obtained by converting the published $\text{H}_2$ masses back to CO luminosities, using the CO-$\text{H}_2$ conversion factor assumed in the respective papers. The Narayanan et al. (2012) and Feldmann, Gnedin & Kravtsov (2012) methods produce very similar results, and when applied to our models both provide very good agreement with the observations. Both clearly produce better agreement with the observations than the fixed CO-$\text{H}_2$ conversion factor. The slope of the relation between CO luminosity and stellar mass varies slightly between the applied CO-$\text{H}_2$ conversion method, however, this is not very well constrained by the data.

Figure 15 shows the CO luminosity function at $z = 0.0$ obtained using the three different CO-$\text{H}_2$ conversion methods. The Feldmann, Gnedin & Kravtsov (2012) method gives the best overall agreement with the observed CO luminosity function. The Narayanan et al. (2012) approach produces similar predictions, but with a slightly shallower low-luminosity end slope and more high CO luminosity galaxies. A fixed conversion factor of $X_{\text{CO}} = 2 \times 10^{20} \text{cm}^{-2} (\text{K km s}^{-1})^{-1}$ overpredicts the observations at all luminosities. All three methods slightly overpredict the number of high-CO luminosity objects.

Figure 16 shows the predicted CO luminosity-functions at redshifts $z = 0.0$–6 for all three applied CO-$\text{H}_2$ conversion methods. We overplot the $z = 0$ CO luminosity function obtained by Keres, Yun & Young (2003) to guide the eye. All three CO-$\text{H}_2$ conversion methods yield qualitatively the same evolutionary trends, but differ more in the details of the predicted evolution. All models predict a relatively mild flattening of the low-luminosity end of the CO luminosity.
Figure 14. CO(1-0) luminosity as a function of stellar mass at $z = 0$ assuming a pressure-based (top row), and metallicity-based (bottom row) $H_2$ formation recipe. We applied a fixed CO-$H_2$ conversion factor (left column), and the prescriptions suggested by Feldmann, Guenin & Kravtsov (2012, center column) and Narayanan et al. (2012, right column) to calculate the conversion from $H_2$ masses to CO (1-0) luminosities. Blue shadings show the conditional probability distribution function $P(L_{CO}|M_*)$ for disc-dominated galaxies, whereas the red solid line shows the median fit. Red triangles and dots are literature values from Leroy et al. (2008) and Saintonge et al. (2011), respectively.

Figure 15. The CO(1-0) luminosity function at $z = 0$ for a pressure- based (left panel) and metallicity-based (right panel) $H_2$ formation model. Different line-styles represent the conversion methods from $H_2$ to CO (1-0), as detailed on the figure. The grey circles and diamonds show the observed CO luminosity functions from Keres, Yun & Young (2003).
function from $z \sim 6.0$, with a more rapid evolution on the bright end. The Feldmann et al. and Narayanan et al. approaches give almost identical results for the low-luminosity end, and differ more at high luminosities. The Feldmann et al. approach predicts fewer high-CO luminosity galaxies at high redshift.

We show the evolution with redshift of the relation between stellar mass and CO luminosity in Figure 17 (assuming the Feldmann et al. and Narayanan et al. approach for the CO-H$_2$ conversion factor). This diagram will, in the near future, be easily filled with observations of the CO luminosity of galaxies from surveys like GOODS, COSMOS, CANDELS using ALMA. As a comparison, we plot observational results presented in Genzel et al. (2010) and Tacconi et al. (2013), color-coded by redshift. We find that our model reproduces the observations very well. There is a clear linear relation between stellar mass and CO luminosity. The slope of this relation does not change with time and only slightly with CO-H$_2$ conversion method. The normalization of the relation does change with time, indicating that the relative amount of CO decreases at the same rate in galaxies spanning a wide range in stellar mass (and type). The Narayanan et al. (2012) CO-H$_2$ conversion method predicts a stronger evolution in the CO luminosities with time, driven by the dependency of the CO-H$_2$ conversion on the H$_2$ surface density. The high surface densities in high-redshift galaxies decrease the CO-H$_2$ conversion factor, increasing the CO luminosity at a given stellar mass. We find only minor differences between the results obtained assuming a pressure- and metallicity-based recipe.

Figure 16. The CO(1-0) luminosity function as a function of redshift assuming a fixed CO-H$_2$ conversion factor (top row), the Feldmann, Gnedin & Kravtsov (2012) approach (center row) and the Narayanan et al. (2012) approach (bottom row) for the conversion between H$_2$ mass and CO (1-0) luminosity. Left and right columns assume a pressure- and metallicity-based H$_2$ formation model, respectively. The grey circles and diamonds show the $z = 0$ observed CO luminosity functions from Keres, Yun & Young (2003).
In this paper we have presented new predictions for the evolution of the multiphase gas content and CO luminosity of galaxies from \( z \sim 6 - 0 \). We apply pressure- (Blitz & Rosolowsky 2006) and metallicity-based (Gnedin & Kravtsov 2010) \( \text{H}_2 \) formation recipes as two different approaches to calculating the molecular fraction of cold gas. Stars are formed following a power-law relation between the surface density of molecular gas and the SFR surface-density (Bigiel et al. 2008). Our goal is to assess the degree to which observations of the gas content of galaxies at high redshift can constrain the physics of the transformation of gas from one phase to another, and the conversion of cold dense gas into stars. In this section we discuss the results of this modelling effort and discuss our findings in comparison with previous studies using similar techniques. We will discuss the agreement and differences between the GK and BR model, draw general conclusions about the evolution of the gas content in galaxies, provide predictions that can help to guide future observational efforts, and discuss our results in the context of the physics driving galaxy formation in general.

We find that both the pressure-based and metallicity-based \( \text{H}_2 \) formation recipes do well at reproducing the gas fractions and gas-to-stellar-mass ratios of local galaxies and the trends with stellar mass and internal galaxy density. There are only very small differences in the scaling relations predicted by the pressure- and metallicity-based recipe over the entire stellar mass range probed. The predicted sizes of atomic hydrogen discs are in good agreement with observations at \( z = 0 \), and the sizes of the modeled \( \text{H}_2 \) discs are in good agreement with observations in the redshift range \( z = 0 - 2 \). We note that these recipes were taken from empirical results calibrated to observations, or from numerical simulations, and were not tuned to cause our semi-analytic model to match these observations. This is an indication that, despite the simplicity of our model for gas partitioning, SF, and disc internal structure, we reproduce the distribution of gas in galaxies with reasonable accuracy.

Both the pressure- and metallicity-based recipe do a fairly good job of reproducing the \( \text{H}_i \) mass function over the whole range probed by observations, with a small excess of high-\( \text{H}_i \) mass galaxies. Both models predict an excess of low-\( \text{H}_i \)-mass galaxies at \( \log (M_{\text{HI}}/M_\odot) < 8 \) compared to observations. The galaxies responsible for the excess at low-\( \text{H}_i \) masses in this model have low stellar masses (\( \log (M_*/M_\odot) \leq 7 \)) and reside in low-mass-halos (\( \log (M_{\text{vir}}/M_\odot) < 9 - 10 \)). This shows that to properly model the smallest galaxies observed in \( \text{H}_i \), it is of key importance to resolve halos down to masses of \( \log (M_{\text{vir}}/M_\odot) \sim 8 \), which frequently has not been possible in previous studies. For example, Somerville et al. (2008b) presented a predicted \( \text{H}_i \)
mass function that was apparently in much better agreement with the observed one, but this was merely an artifact of the relatively coarse halo mass resolution ($10^{10} M_{\odot}$) adopted in their simulations. Both recipes successfully predict the H$_2$ mass function over the entire mass range probed.

In both models, the number density of H$_i$-massive galaxies shows an increase of about an order of magnitude from $z \sim 6$ to 4, then remains nearly constant to $z \sim 0$. This result indicates that there is a kind of self-regulated equilibrium that arises naturally in these models. To first order, the constant high-mass end of the H$_i$ mass function in our models is a consequence of the balance between accretion and the transformation of H$_2$ into H$_i$. Observations have shown that H$_i$ saturates at surface densities of $\Sigma_{\text{H}_i} = 6 - 10 M_{\odot} \text{pc}^{-2}$ and that higher cold gas densities are dominated by H$_2$ (Blitz & Rosolowsky 2006; Leroy et al. 2008). In our models, as new gas is accreted, the amount of gas that is above surface densities where H$_2$ formation is efficient increases, leading to conversion of H$_i$ into H$_2$. The constant high-mass end of the H$_i$ mass function is a strong prediction that can be tested by the VLA up to $z \lesssim 0.4$ (Fernández et al. 2013), and SKA and its pathfinders ASKAP and MeerKat in the near future. It will not only probe the H$_2$ formation recipes, but also the physics that drives the accretion, consumption, and heating and/or ejection of cold gas from galaxies.

The number density of low H$_2$-mass galaxies shows a strikingly different evolution, decreasing almost monotonically from $z \sim 4$ to $z \sim 0$. This behavior is qualitatively very similar in the two H$_2$ formation models. It is intriguing that this behavior — weak evolution of massive objects, with a decrease in the number of low-mass objects — is qualitatively similar to the evolution of the observed stellar mass function (Cimatti, Daddi & Renzini 2006; Marchesini et al. 2009), sometimes referred to as “mass assembly downsizing”. This suggests that “mass assembly downsizing” may be linked to the evolution of the molecular gas content of galaxies and the ability to form stars out of this molecular gas.

We also find only minor differences in the evolution of the gas fraction. Gas fractions are quite high ($\geq 0.7$) over a broad range of stellar masses ($10^8 \lesssim M_* \lesssim 10^{12} M_{\odot}$) from $z \sim 6$ to 3, then drop fairly rapidly at lower redshifts. This drop in gas fraction occurs at higher redshift for galaxies with higher stellar mass — massive galaxies appear to consume or expel their gas earlier than less massive galaxies. A similar trend holds for the H$_2$ fraction of galaxies, but the rate at which the H$_2$ fraction drops is even faster than the rate of decline of the overall cold gas fractions. These trends are a different manifestation of mass assembly downsizing, and are in qualitative agreement with the observed evolution in galaxy gas fractions (Tacconi et al. 2010; Magdis et al. 2012; Narayanan et al. 2012; Popping et al. 2012; Tacconi et al. 2013; Sargent et al. 2013). Future surveys of the molecular gas content of galaxies, as well as future efforts to indirectly estimate the gas content of galaxies, will be able to probe the gas content in galaxies over a much wider range in galaxy properties and environment, improving the constraints that can be obtained on models of galaxy formation.

In a picture where galaxy gas fractions represent the competition between gas inflow, outflow and consumption through star formation (Davé, Finlator & Oppenheimer 2011), the decreasing gas fractions below redshifts of $z = 3$ indicate that outflows and gas consumption largely dominate this competition. Galaxies run out of cold gas and of molecular gas, but not necessarily at the same rate (Popping et al. 2012). Taking into account that galaxies form their stars out of molecular gas, this means that declining SFRs are not only due to a decline in the cold gas available, but also due to an even more rapid decline of the H$_2$ fraction of gas.

The relative H$_2$ content of galaxies with stellar masses below $10^{10} M_{\odot}$ predicted by our models appears to be slightly too low in the redshift regime $1.0 < z < 2.0$ compared to the predictions by Popping et al. (2012). This effect is still present after taking selection criteria into account. It is probably related to the low-mass galaxy problem in models of galaxy formation, where galaxies in this mass regime are too passive at these redshifts with respect to the observations. We find that the low H$_2$ content in these galaxies might be driving this problem, leading to inefficient star formation. A successful solution to the low-mass galaxy problem must also produce higher gas fractions in low-mass galaxies at intermediate redshift.

The predictions of the cosmic-density evolution of H$_i$, H$_2$ and the total cold gas budget show the largest differences between pressure- and metallicity-based H$_2$ recipes. The metallicity-based recipe yields a much higher cosmic density of cold gas and the density peaks at lower redshift. More striking is the difference in the evolution of the global H$_2$ fraction, $\Omega_{\text{HI}}/\Omega_{\text{gas}}$. The global H$_2$ fraction assuming a metallicity-based H$_2$ formation recipe shows only a mild decrease of a factor of $\sim 2$ from $z \sim 6$ to 0, whereas a pressure-based recipe predicts a strong decrease of a factor $\sim 6$ over this redshift range. Our predicted cosmic density of H$i$ $\Omega_{\text{HI}}$ is, at face value, in poor agreement with estimates from observations of DLAs for both H$_2$ prescriptions. However, we have presented $\Omega_{\text{HI}}$ for all galaxies without taking into account the selection criteria for DLAs.

It is important to note that here we have computed the global density of gas by adding up all the gas in galaxies. However, DLAs may not provide an unbiased estimate of the total H$i$ content of the Universe. Berry et al. (2013) present a detailed analysis of predicted DLA properties using the same semi-analytic models presented here, and show that $\Omega_{\text{HI}}$ derived from DLAs as in the observational estimates shown here can differ substantially from the “true” underlying $\Omega_{\text{HI}}$. They argue that a greater fraction of DLAs may arise from intergalactic or circumgalactic gas at $z \gtrsim 3$, while at lower redshifts, a large amount of H$i$ may be in galaxies that have column densities too low for them to be selected as DLAs, leading to very weak evolution in $\Omega_{\text{DLA}}$, as observed.

The significant differences between the metallicity- and pressure-based recipes for H$_2$ formation all find their origin in low mass galaxies ($\log (M_*/M_{\odot}) < 9$) within low mass halos ($\log (M_{\text{ halo}}/M_{\odot}) < 10$). A significant fraction of the cold gas and H$i$ that leads to the higher cosmic densities of these quantities in the model with the metallicity-based recipe is within virtually “pristine” halos that contain less than $10^8 M_{\odot}$ of stars (see also the discussion in Berry et al. 2013). These differences are driven by a lack of metals at high redshift, necessary for the metallicity-based recipe to form molecular gas. As a result fewer stars form, less gas
is consumed and the cold gas content of galaxies piles up. Furthermore, the lack of formed stars slows down the production of metals necessary to form H$_2$. Meanwhile, the high internal densities of high-redshift galaxies are highly conducive to the formation of molecules through a pressure-based recipe. It is important to note that both the pressure- and metallicity-based recipes predict a small excess of low-HI-mass galaxies. None of the various H$_2$ formation recipes that we have explored are able to remove this excess, suggesting that it may arise from other physical processes.

We present predictions for the CO luminosities of our modelled galaxies using different methods to estimate the conversion between CO and H$_2$. Although the general trends in CO are similar, different approaches to estimating the CO-H$_2$ conversion factor yield different predictions in detail, especially for lower-H$_2$-mass galaxies. The use of a fixed conversion factor between CO and H$_2$ in our models overpredicts the observed luminosity function over a wide range of CO luminosities, although a different value for $X_{\text{CO}}$ can change the normalization of the luminosity function. Using either the Narayanan et al. (2012) or Feldmann, Gnedin & Kravtsov (2012) CO-H$_2$ conversion prescriptions, which depend on galaxy properties, we obtain good agreement with the observed H$_2$ luminosity function below the knee, but overpredict the number of high-H$_2$ mass galaxies by a significant amount, more so with the Narayanan et al. (2012) prescription. The predicted evolution of the CO luminosity function is qualitatively similar to that of the H$_2$ luminosity function, described above, although the detailed predictions depend somewhat on the adopted conversion prescription. Future surveys with sub-mm and radio telescopes such as the ALMA, PdBI, LMT, VLA, ATCA, and SKA, will be able to probe the CO $J = 1 - 0$ luminosity function at $z > 2$ and provide valuable constraints for our models.

4.1 Comparison with previous work

We now discuss our results with respect to other recent theoretical predictions of the evolution of atomic and molecular gas in semi-analytic galaxy formation models. We will attempt to not only point out the differences between the various modeling efforts, but also the common results that can shed more light on the physics at play in galaxy formation. We used the fitting functions provided by Gnedin & Kravtsov (2011, GK) in our metallicity-based recipe for the formation of H$_2$, whereas most previous modeling efforts have used the analytic model of Krumholz, McKee & Tumlinson (2009). These two approaches have been compared and were found to be very similar except at the lowest metallicities (Krumholz & Gnedin 2011). We will show an explicit comparison of the two approaches in SPT14, and also find that they produce similar results. The GK fitting functions appear to be somewhat more robust and produce better agreement with observations, which is why we adopt them. Another difference in our approach is that we have separated the recipes for partitioning gas into an atomic and molecular component, and those for converting molecular gas into stars, while in some previous works both recipes were varied, making it more difficult to identify which aspects of the recipes may be causing differences in the results. In SPT14, we will present a systematic study of the effects of varying both the gas partitioning and star formation recipes separately. Here, we leave the star formation recipe fixed and vary only the gas partitioning recipes.

A first attempt to study the atomic and molecular hydrogen content of galaxies was presented in Obreschkow et al. (2009a) and Obreschkow & Rawlings (2009a). The authors use the semi-analytic predictions from De Lucia & Blaizot (2007) and calculate the H$_2$ and HI content of galaxies in post-processing using the Blitz & Rosolowsky (2006) pressure-based formalism. This model does not include an H$_2$ based star-formation recipe, but rather assumes a traditional “total gas” based Kennicutt star formation relation, where stars form above some critical cold gas surface density. Obreschkow et al. (2009a) and Obreschkow & Rawlings (2009a) find HI and H$_2$ mass functions, H$_2$ disc sizes and an evolution in universal density of H$_2$ (Fig. 13) very similar to our findings when we assume a pressure based H$_2$ formation recipe, and an H$_2$-based star-formation recipe.

Obreschkow et al. (2009b) estimate the CO luminosity (ranging from CO $J=1$-0 to CO $J=10$-9) of a galaxy from its gas temperature based on the SFR surface density or AGN bolometric luminosity under local thermodynamic equilibrium (i.e. a single gas phase). The authors find that the low-luminosity end of the CO $J=1$-0 luminosity function is already in place at $z = 2$, contrary to our predictions. The evolution of the bright end of the CO $J=1$-0 luminosity function is in much better agreement with our results. Obreschkow et al. (2009b) point out that above $z > 1$ the CMB starts to act as a bright background reducing the observed CO $J=1$-0 luminosity. At the same time, the higher excitation temperatures of the warm CMB in the early universe will ease the observability of CO emission (Combes, Maoli & Omont 1999; Gnedin, Silk & Spaans 2001), although the negative effect of the CMB dominates. These are effects we did not include in our model but which can play a significant role when observing young galaxies in the early universe. In particular, sources at $z > 5$ without a strong heating by a starburst or AGN will not be detectable through low CO transitions.

Lagos et al. (2011a,b) study the evolution of the atomic and molecular gas content of galaxies using a pressure- and metallicity based H$_2$ recipe in a semi-analytic model of galaxy formation. Their pressure-based model uses an H$_2$-prescription from Blitz & Rosolowsky (2006) and a star-formation model from Leroy et al. (2008), very similar to our pressure-based model. Their metallicity-based model follows the H$_2$ prescription and star-formation model presented in Krumholz, McKee & Tumlinson (2009). Although the authors vary the star-formation relation in their models, the models are not calibrated to necessarily fit the $z = 0$ luminosity functions, stellar and gas mass fractions and mass functions. The authors find that the metallicity-based recipes fail to reproduce the observed HI-mass functions and select the pressure-based recipes in combination with the Bower et al. (2006) semi-analytic model as their preferred model. Taking into account that the Lagos et al. (2011b) models are not calibrated to match local observations, we argue that a metallicity-based H$_2$ and star-formation recipe should not be considered ruled out, although we also find (to a much lesser extent) that the metallicity-based H$_2$ recipe tends to produce too many low-HI mass galaxies at $z = 0$. The KMT model is known to break down at the lowest metallicities, due to a failure of the assumption of chemi-
In the metallicity-based models, the results can also be somewhat sensitive to the treatment of this “seed” metallicity, which may be provided by Pop III stars.

Using their preferred model, Lagos et al. (2011a) find an evolution in the HI and H$_2$ mass functions, gas fractions and H$_2$ density of the universe very similar to our results. The authors find a bump in the HI mass function at log (M$_{HI}$/h$^{-2}$M$_{⊙}$) $\sim$ 7.5 − 8.0, similar to (although much larger than) the excess number of low-HI-mass galaxies we find. They ascribe this excess to a mismatch between the observed and modeled radii of the galaxy discs. We, however, have shown the sizes of the gas discs in our models (including the sizes of the HI and H$_2$ components separately) are in good agreement with observations, so we do not think this is the main cause of the remaining excess of intermediate HI-mass galaxies in our models, though it may partially explain the better agreement of our metallicity-based model with observations. Lagos et al. (2011a) finds a good match between their preferred model and the observed CO luminosity function by Keres, Yun & Young (2003). To obtain this match the authors need to assume a fixed CO-to-H$_2$ conversion factor of $X = 3.5 \times 10^{-20}$cm$^{-2}$/Kkm$s^{-1}$.

Fu et al. (2012) also studied the redshift evolution of atomic and molecular gas in galaxies, although the emphasis of their work lies more on the evolution of the mass-metallicity relation. In their work the authors use a variety of star-formation models (including the Bigiel et al. 2008 recipe) and apply both a metallicity- (based on Krumholz, McKee & Tumlinson 2009) and a pressure-based H$_2$ recipe (based on Blitz & Rosolowsky 2006). Their model is calibrated to the local HI, H$_2$ and stellar mass functions. The authors find that the evolution of the atomic and molecular gas fraction of galaxies is very similar for both applied H$_2$ prescriptions, and is more dependent on the star-formation model. Similar to our findings, their results suggest that $\Omega_{H_2}/\Omega_{HI}$ increases monotonically with increasing redshift for the pressure-based H$_2$ recipe, whereas it decreases at redshifts $z > 3$ for the metallicity-based recipe. The resolution of the models in Fu et al. (2012) is not sufficient to study the differences in behavior of the low mass end of the HI and H$_2$ mass function for the pressure- and metallicity based H$_2$ recipes. This makes it difficult to compare our excess in low-HI-mass galaxies and our constraints on the different H$_2$ formation recipes with the results of Fu et al. (2012).

Despite the different implementations of the physical recipes, the three discussed models and ours all agree that a pressure-based recipe for H$_2$ formation predicts a monotonic increase for $\Omega_{H_2}/\Omega_{HI}$ with redshift (Fig. 13, although note the decline in $\Omega_{H_2}/\Omega_{HI}$ for the Lagos et al. 2011a, model), whereas it flattens out for a metallicity based recipe. We therefore conclude that the applied H$_2$ recipe is likely to be responsible for these trends. As discussed extensively in the previous subsection, in the metallicity-based models, the low metallicities at early times make H$_2$ formation and hence star formation very inefficient, in spite of the higher gas densities. Thus star formation, H$_2$ formation, and enrichment are delayed in these models relative to the pressure-based models.

5 CONCLUSIONS

We have presented predictions for the evolution of the atomic and molecular hydrogen content of galaxies from $z \sim 6 − 0$, based on a semi-analytic model of galaxy formation, including new modeling of the partitioning of cold gas in galactic discs into atomic, molecular, and ionised phases. We present results for two different H$_2$ formation recipes: one a pressure-based recipe motivated by the empirical relation between molecular fraction and gas midplane-pressure from Blitz & Rosolowsky (2006), and one based on numerical hydrodynamic simulations in which the molecular fraction is highly dependent on the cold gas metallicity as well as the local UV background (Gnedin & Kravtsov 2011). We compared our predictions to local and high-redshift observations and adopted an alternate approach in which we estimate the CO content of galaxies and compare directly with CO observations. We summarize our main findings below.

- Without any tuning, our models correctly predict the trends between gas fractions and gas-to-stellar-mass ratios of HI and H$_2$ in local galaxies with mass and internal density. We furthermore reproduce the HI and H$_2$ disc sizes of local and high redshift galaxies.
- Both H$_2$ formation recipes reproduce the observed $z = 0$ HI mass function fairly well over the whole range probed by observations. Both models predict a small excess of low-HI-mass galaxies. The high-mass end of the HI mass function remains remarkably constant at redshifts of $z \lesssim 2.0$ for both H$_2$ formation recipes.
- Both recipes correctly predict the H$_2$ mass function over the entire mass range probed. The number density of H$_2$-massive galaxies increases from $z \sim 6$ to $z \sim 4.0$ after which it remains fairly constant, whereas the number density of low-H$_2$ mass galaxies decreases almost monotonically from $z \sim 4$ to $z \sim 0$.
- Galaxy gas fractions remain relatively high ($\gtrsim 0.7$) from $z \sim 6 − 3$, then drop fairly rapidly. A similar trend holds for the $H_2$ fraction of galaxies, but the drop occurs at an even higher rate.
- The metallicity-based recipe yields a much higher cosmic density of cold gas over the entire redshift range probed. The cosmic H$_2$ fraction as predicted by the metallicity-based recipe is much lower than the H$_2$ fraction predicted by the pressure-based recipe.
- The galaxies responsible for the high cosmic gas density and low cosmic H$_2$ fraction all reside in low-mass halos (log (M$_{halo}$/M$_{⊙}$) < 10), and contain negligible amounts of stellar material. The build-up of atomic gas in these low-mass halos is driven by a lack of metals at high redshift, necessary to form molecular gas, stars, and produce more metals.
- The conversion of H$_2$ masses to CO luminosities provides valuable direct predictions for future surveys with ALMA at low redshifts or radio interferometers such as the VLA at higher redshifts. None of the presented methods for the CO-to-H$_2$ conversion predicts perfect agreement with
observations from the literature, although the physically mottled nature of the Narayanan et al. (2012) and Feldmann, Gnedin & Kravtsov (2012) approaches are favoured over a constant CO-to-H$_2$ conversion factor.

The results presented in this paper can serve as predictions for future surveys of the atomic and molecular content of galaxies. We look forward to observations from new and upcoming facilities, that will be able to confront our predictions, further constraining the physics that drives the formation of molecules and the evolution of gas in galaxies.

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References

Baugh C. M., Lacey C. G., Frenk C. S., Granato G. L., Silva L., Bressan A., Benson A. J., Cole S., 2005, MNRAS, 356, 1191
Berry M., Somerville R. S., Haas M. R., Gawiser E., Maller A., Popping G., Trager S. C., 2013, ArXiv e-prints: 1308.2598
Bigiel F., Leroy A., Walter F., Brinks E., de Blok W. J. G., Madore B., Thornley M. D., 2008, AJ, 136, 2846
Bigiel F. et al., 2011, ApJ, 730, L13+
Birnboim Y., Dekel A., 2003, MNRAS, 345, 349
Blitz L., Rosolowsky E., 2006, ApJ, 650, 933
Blumenthal G. R., Faber S. M., Flores R., Primack J. R., 1986, ApJ, 301, 27
Bolatto A. D., Leroy A. K., Rosolowsky E., Walter F., Blitz L., 2008, ApJ, 686, 948
Bondi H., 1952, MNRAS, 112, 195
Booth R. S., de Blok W. J. G., Jonas J. L., Fanaroff B., 2009, ArXiv e-prints
Boselli A., Cortese L., Boquien M., Boissier S., Catinella B., Lagos C., Saintonge A., 2014, ArXiv e-prints
Bothwell M. S. et al., 2013, MNRAS, 563
Bower R. G., Benson A. J., Malbon R., Helly J. C., Frenk C. S., Baugh M. C., Cole S., Lacey C. G., 2006, MNRAS, 370, 645
Boylan-Kolchin M., Ma C.-P., Quataert E., 2008, MNRAS, 383, 93
Braun R., 2012, ApJ, 749, 87
Bromm V., Larson R. B., 2004, ARA&A, 42, 79
Carilli C. L., Rawlings S., 2004, New A Rev., 48, 979
Casey C. M. et al., 2011, MNRAS, 415, 2723
Catinella B., Haynes M. P., Giovanelli R., Gardner J. P., Connolly A. J., 2008, ApJ, 685, L13
Catinella B. et al., 2013, ArXiv e-prints: 1308.1676 —, 2012, A&A, 544, A65 —, 2010, MNRAS, 403, 683
Christensen C., Quinn T., Governato F., Stilp A., Shen S., Wadsley J., 2012, MNRAS, 425, 3058
Cimatti A., Daddi E., Renzini A., 2006, A&A, 453, L29
Cole S., Aragon-Salamanca A., Frenk C. S., Navarro J. F., Zepf S. E., 1994, MNRAS, 271, 781
Cole S., Lacey C. G., Baugh C. M., Frenk C. S., 2000, MNRAS, 319, 168
Combes F., Moaïl R., Omont A., 1999, A&A, 345, 369
Croton D. J. et al., 2006, MNRAS, 365, 11
Daddi E. et al., 2010, ApJ, 713, 686
Davé R., Finlator K., Oppenheimer B. D., 2011, MNRAS, 416, 1354
Davé R., Finlator K., Oppenheimer B. D., Fardal M., Katz N., Keres D., Weinberg D. H., 2010, MNRAS, 404, 1355
De Lucia G., Blaizot J., 2007, MNRAS, 375, 2
Dekel A., Birnboim Y., 2006, MNRAS, 368, 2
Dutton A. A., van den Bosch F. C., Dekel A., 2010, MNRAS, 405, 1690
Elmegreen B. G., 1989, ApJ, 338, 178
—, 1993, ApJ, 411, 170
Erb D. K., Steidel C. C., Shapley A. E., Pettini M., Reddy N. A., Adelberger K. L., 2006, ApJ, 646, 107
Feldmann R., Gnedin N. Y., Kravtsov A. V., 2012, ApJ, 747, 124
Ferrández X. et al., 2013, ApJ, 770, L29
Flores R., Primack J. R., Blumenthal G. R., Faber S. M., 1993, ApJ, 412, 443
Fontanot F., De Lucia G., Monaco P., Somerville R. S., Santini P., 2009, MNRAS, 397, 1776
Forster Schreiber N. M. et al., 2009, ApJ, 706, 1364
—, 2006, ApJ, 645, 1062
Fu J., Guo Q., Kauffmann G., Krumholz M. R., 2010, MNRAS, 409, 515
Fu J., Kauffmann G., Li C., Guo Q., 2012, MNRAS, 424, 2701
Genzel R. et al., 2010, MNRAS, 407, 2091
Giovanelli R. et al., 2005, AJ, 130, 2598
Glover S., 2013, in Astrophysics and Space Science Library, Vol. 396, Astrophysics and Space Science Library, Wildtind T., Mobasher B., Bromm V., eds., p. 103
Glover S. C. O., Mac Low M.-M., 2011, MNRAS, 412, 337
Gnedin N. Y., 2000, ApJ, 542, 535
—, 2012, ApJ, 754, 113
Gnedin N. Y., Kravtsov A. V., 2010, ApJ, 714, 287
—, 2011, ApJ, 728, 88
Gnedin N. Y., Silk J., Spaans M., 2001, ArXiv Astrophysics e-prints: 0106110
Greif T. H., Glover S. C. O., Bromm V., Klessen R. S., 2010, ApJ, 716, 510
Grogin N. A. et al., 2011, ApJS, 197, 35
Guzmán R., Petitjean P., de Carvalho R. R., Djorgovski S. G., Noterdaeme P., Castro S., Poppe P. C. D. R., Aghae A., 2009, A&A, 508, 133
Guo Q. et al., 2011, MNRAS, 413, 101
Guo Q., White S., Li C., Boylan-Kolchin M., 2010, MNRAS, 404, 1111
Haiman Z., Loeb A., 1996, ApJ, 467, 522
Heller T. T., Tornberg M. D., Regan M. W., Wong T., Sheth K., Vogel S. N., Blitz L., Bock D., 2003, ApJS, 145, 259
Hopkins P. F., Cox T. J., Younger J. D., Hernquist L., 2009a, ApJ, 691, 1168

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Evolution of atomic and molecular gas in galaxies

Hopkins P. F. et al., 2009b, MNRAS, 397, 820
Hunter D. A. et al., 2012, AJ, 144, 134
Johnston S. et al., 2008, Experimental Astronomy, 22, 151
Kang X., Jing Y. P., Silk J., 2006, ApJ, 648, 820
Kauffmann G., Colberg J. M., Diaferio A., White S. D. M., 1999, MNRAS, 303, 188
Kauffmann G., White S. D. M., Guiderdoni B., 1993, MNRAS, 264, 201
Kennicutt, Jr. R. C., 1998, ApJ, 498, 541
Keres D., Yuan M. S., Young J. S., 2003, ApJ, 582, 659
Kereˇ s D., Katz N., Weinberg D. H., Dav´ e R., 2005, MNRAS, 363, 2
Koekemoer A. M. et al., 2011, ApJS, 197, 36
Komatsu E. et al., 2009, ApJS, 180, 330
Kravtsov A. V., 1999, PhD thesis, NEW MEXICO STATE UNIVERSITY
Kravtsov A. V., Berlind A. A., Wechsler R. H., Klypin A. V., 1999, MNRAS, 303, 188
Kravtsov A. V., Berlind A. A., Gottl¨ ober S., Allgood B., Primack J. R., 2004, ApJ, 609, 35
Krumholz M. R., Dekel A., 2012, ApJ, 753, 16
Krumholz M. R., Gnedin N. Y., 2011, ApJ, 729, 36
Krumholz M. R., McKee C. F., Tumlinson J., 2008, ApJ, 689, 865
—, 2009, ApJ, 693, 216
Kuhlen M., Krumholz M. R., Madau P., Smith B. D., Wise J., 2012, ApJ, 749, 36
Lagos C. D. P., Baugh C. M., Lacey C. G., Benson A. J., Kim H.-S., Power C., 2011a, MNRAS, 1776
Lagos C. d. P., Bayet E., Baugh C. M., Lacey C. G., Bell T. A., Fanidakis N., Geach J. E., 2012, MNRAS, 426, 2142
Lagos C. D. P., Lacey C. G., Baugh C. M., Bower R. G., Benson A. J., 2011b, MNRAS, 416, 1566
Leroy A. K. et al., 2009, AJ, 137, 4670
Leroy A. K., Walter F., Brinks E., Bigiel F., de Blok W. J. G., Madore B., Thornley M. D., 2008, AJ, 136, 2782
Magdis G. E. et al., 2012, ApJ, 760, 6
Mannucci F. et al., 2009, MNRAS, 398, 1915
Marchesini D., van Dokkum P. G., F¨ urster Schreiber N. M., Franx M., Labb´ e I., Wuyts S., 2009, ApJ, 701, 1765
Martin A. M., Papastergis E., Giovanelli R., Haynes M. P., Springob C. M., Stierwalt S., 2010, ApJ, 723, 1359
McKee C. F., Ostriker E. C., 2007, ARA&A, 45, 565
Menci N., Fontana A., Giallongo E., Grazian A., Salimbeni S., 2006, ApJ, 647, 753
Mo H. J., Mao S., White S. D. M., 1998, MNRAS, 295, 319
Monaco P., Fontanot F., Taffoni G., 2007, MNRAS, 375, 1189
Murray N., Rahman M., 2010, ApJ, 709, 424
Namazu F., Umemura M., 2001, ApJ, 548, 19
Narayanan D., Bothwell M., Dav´ e R., 2012, MNRAS, 426, 1178
Narayanan D., Krumholz M. R., Ostriker E. C., Hernquist L., 2012, MNRAS, 421, 3127
Narvaro J. F., Frenk C. S., White S. D. M., 1996, ApJ, 462, 563
Niemel¨ a-S., Somerville R. S., Ferguson H. C., Huang K.-H., Lotz J., Koekemoer A. M., 2012, MNRAS, 421, 1539
Noterdaeme P. et al., 2012, A&A, 547, L1
Obreschkow D., Croton D., De Lucia G., Khochfar S., Rawlings S., 2009a, ApJ, 698, 1467
Obreschkow D., Heywood I., K¨ lockner H.-R., Rawlings S., 2009b, ApJ, 702, 1321
Obreschkow D., Rawlings S., 2009a, ApJ, 696, L129
—, 2009b, MNRAS, 394, 1857
Ostriker E. C., McKee C. F., Leroy A. K., 2010, ApJ, 721, 975
Pelupessy F. I., Papadopoulos P. P., van der Werf P., 2006, ApJ, 645, 1024
P´ eroux C., Dessauges-Zavadsky M., D’Odorico S., Sun Kim T., McMahon R. G., 2005, MNRAS, 363, 479
Popping G., Caputi K. I., Somerville R. S., Trager S. C., 2012, MNRAS, 425, 2386
Popping G., Perez-Beaupuits J. P., Spaans M., Trager S. C., Somerville R. S., 2013, ArXiv e-prints: 1310.1476
Power C., Baugh C. M., Lacey C. G., 2010, MNRAS, 406, 43
Prochaska J. X., Wolfe A. M., 2009, ApJ, 696, 1543
Rao S. M., Turnshek D. A., Nestor D. B., 2006, ApJ, 636, 610
Riechers D. A., Hodge J., Walter F., Carilli C. L., Bertoldi F., 2011, ApJ, 739, L31
Robertson B., Cox T. J., Hernquist L., Franx M., Hopkins P. F., Martini P., Springel V., 2006, ApJ, 641, 21
Robertson B. E., Kravtsov A. V., 2008, ApJ, 680, 1083
Rohitaille T. P., Whitney B. A., 2010, ApJ, 710, L11
Saintonge A. et al., 2011, MNRAS, 415, 32
—, 2012, ApJ, 758, 73
Sargent M. T. et al., 2013, ArXiv e-prints: 1303.4392
Schmidt M., 1959, ApJ, 129, 243
Schneider R., Ferrara A., Natarajan P., Omukai K., 2002, ApJ, 571, 30
Schuba A. et al., 2011, AJ, 142, 37
Sofion M. P., Rivolo A. R., Barrett J., Yahil A., 1987, ApJ, 319, 730
Somerville R. S. et al., 2008a, ApJ, 672, 776
Somerville R. S., Gilmore R. C., Primack J. R., Dom´ ınguez A., 2012, MNRAS, 423, 1992
Somerville R. S., Hopkins P. F., Cox T. J., Robertson B. E., Hernquist L., 2008b, MNRAS, 391, 481
Somerville R. S., Kolatt T. S., 1999, MNRAS, 310, 1087
Somerville R. S., Hopkins P. F., Martini P., Springel V., 2006, ApJ, 641, 21
Somerville R., Primack J. R., Dom´ ınguez A., 2012, MNRAS, 423, 1992
Tacconi L. J. et al., 2010, Nature, 463, 781
Tolstoy E., Hill V., Tosi M., 2009, ArXiv e-prints: 0907.0468
Tumlinson J., 2008a, MNRAS, 394, 1857
Verheijen M. A. W., Sancisi R., 2001, MNRAS, 1776
Verheijen M. A., Franx M., 2000, MNRAS, 702, 1321
Walter F., Brinks E., de Blok W. J. G., Bigiel F., Kennicutt R. C., 2008, AJ, 136, 2563
Weinmann S. M., Pasquali A., Oppenheimer B. D., Finlator K., Mendel J. T., Crain R. A., Macci` o A. V., 2012, MNRAS, 426, 2797
Wise J. H., Turk M. J., Norman M. L., Abel T., 2012, ApJ, 745, 50
Wong T., Blitz L., 2002, ApJ, 569, 157
Wootten A., Thompson A. R., 2009, IEEE Proceedings, 97, 1463
Zafar T., Péroux C., Popping A., Milliard B., Deharveng J.-M., Frank S., 2013, A&A, 556, A141
Zwaan M. A., Meyer M. J., Staveley-Smith L., Webster R. L., 2005, MNRAS, 359, L30