

The role of the H_2 adiabatic index in the formation of the first stars

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ABSTRACT

The adiabatic index of H_2 (γ_{H_2}) is non-constant at temperatures between 100 and 10^4 K due to the large energy spacing between its rotational and vibrational modes. For the formation of the first stars at redshifts 20 and above, this variation can be significant because primordial molecular clouds are in this temperature range due to the absence of efficient cooling by dust and metals. We study the possible importance of variations in γ_{H_2} for the primordial initial mass function by carrying out 80 3D gravitohydrodynamic simulations of collapsing clouds with different random turbulent velocity fields, half using fixed $\gamma_{H_2} = 7/5$ in the limit of classical diatomic gas (used in earlier works) and half using an accurate quantum mechanical treatment of γ_{H_2} . We use the adaptive mesh refinement code FLASH with the primordial chemistry network from KROME for this study. The simulation suite produces almost 400 stars, with masses from 0.02 to $50 M_\odot$ (mean mass $\sim 10.5 M_\odot$ and mean multiplicity fraction ~ 0.4). While the results of individual simulations do differ when we change our treatment of γ_{H_2} , we find no statistically significant differences in the overall mass or multiplicity distributions of the stars formed in the two sets of runs. We conclude that, at least prior to the onset of radiation feedback, approximating H_2 as a classical diatomic gas with $\gamma_{H_2} = 7/5$ does not induce significant errors in simulations of the fragmentation of primordial gas. None the less, we recommend using the accurate formulation of the H_2 adiabatic index in primordial star formation studies since it is not computationally more expensive and provides a better treatment of the thermodynamics.

Key words: hydrodynamics – turbulence – stars: formation – stars: Population III – early Universe – primordial nucleosynthesis.

1 INTRODUCTION

Stars are usually classified into three populations based on their metal content (Bond 1981; McDowell 1986). The generation of stars with the highest metallicity is known as Population I. Population II corresponds to stars that have relatively less metal content, and Population III is the hypothetical limit of stars that have no metals. Population III stars, also known as first stars, are believed to have formed in dust-free environments out of primordial species produced by the big bang (Saslaw & Zipoy 1967; Galli & Palla 1998). They are further classified into Population III.1 (the first generation of stars) and Population III.2 (primordial stars affected by radiation from other stars; see McKee & Tan 2008; De Souza, Yoshida & Ioka 2011). While contemporary star formation is well studied thanks to observations and simulations, the formation of the first generation of stars in the Universe still remains a mystery

because of the lack of direct observations at spatially resolved scales beyond $z > 11.1$ (Oesch et al. 2016), and of zero-metallicity stars, if any, in the Local Group (Griffen et al. 2018; Hartwig et al. 2019).

The first stars are believed to have formed between redshifts $15 \leq z \leq 30$ (see reviews by Abel, Bryan & Norman 2002; Bromm & Larson 2004; Glover 2005; Ciardi & Ferrara 2005; Bromm 2013; Karlsson, Bromm & Bland-Hawthorn 2013), at the centre of dark matter minihaloes that have high baryonic densities of the order of $\sim 10^4 \text{ cm}^{-3}$ (Abel et al. 2002; Bromm, Coppi & Larson 2002). By this epoch, the first clouds of neutral hydrogen had formed after recombination (Peebles 1968). Since the first clouds only contained primordial elements (H, He, Li, and their isotopes), cooling during the collapse is inefficient as compared to contemporary star formation where dust and metal lines are present (Omukai et al. 2005; Bromm 2013).

Early simulations of the first stars did not have a long dynamical range in time and thus could not follow the large-scale evolution once the primordial clouds started to collapse. They showed no fragmentation, leading to the belief that the first stars were very

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massive and evolved in isolation (Abel et al. 2002; Bromm et al. 2002; Yoshida et al. 2006). Once numerical techniques were improved to include modules like sink particles and work with better and more efficient solvers, it became possible to simulate farther in time past the initial collapse. Since then, fragmentation has been observed in almost all simulations of the first stars (e.g. Clark et al. 2011a; Stacy, Greif & Bromm 2012; Hirano et al. 2014, 2015). However, it occurs very close to the central protostar, on scales as small as a few au (Kratter & Matzner 2006; Susa, Hasegawa & Tominaga 2014; Klessen 2018). This is because of the lack of an adiabatic core larger than 1 au even before protostar formation, as is observed in simulations of contemporary star formation (Larson 1969; Bate 1998). Thus, in the case of the first stars, the circumstellar disc grows gradually and fragmentation occurs near the central protostar. The observation that primordial gas clouds do fragment naturally raises the question of what initial mass function (IMF) this process yields. Determining the IMF of first stars has thus become a central goal of modern first star research (Tumlinson, Venkatesan & Shull 2004; Schneider et al. 2006; Susa 2013; Susa et al. 2014; Ishigaki et al. 2018).

In this work, we investigate the sensitivity of this IMF and closely related quantities such as the multiplicity statistics of first stars to the thermodynamics of molecular hydrogen. This molecule controls the thermal and chemical evolution of collapsing primordial clouds and becomes the dominant chemical state of hydrogen once the density is high enough. While there has been extensive work on the importance of H_2 as a coolant, no published 3D simulations of first star fragmentation to date have systematically investigated another potential role it might play in controlling fragmentation, via the dependence of the adiabatic index on the H_2 mass fraction and temperature.

The adiabatic index is potentially important to the IMF because it determines how easy or hard it is to compress the gas, and thus how much the gas resists fragmentation. A gas with higher γ is more resistant to fragmentation because, for the same level of pressure fluctuation, it will respond with a smaller density fluctuation than a gas with lower γ . In the context of contemporary star formation, Boley et al. (2007) show that simulations of gravitationally unstable protoplanetary discs using a correct quantum treatment of γ_{H_2} produce qualitatively different amounts of fragmentation than those where γ_{H_2} is approximated as constant; Bitsch, Boley & Kley (2013) show that there are also differences in the subsequent accretion and migration of the fragments. Vaytet, Tomida & Chabrier (2014) show that variations in γ_{H_2} lead to changes in the dynamics of the first Larson (1969) cores that result from collapse. Gravitationally unstable discs seem particularly sensitive to the adiabatic index of the gas, and this is precisely the mode of fragmentation that determines the IMF of the first stars. Moreover, first star formation occurs in gas clouds at temperatures of hundreds of Kelvin (Omukai et al. 2005), which is precisely the temperature range at which the ro-vibrational modes of H_2 first become excited, and thus the departure from classical behaviour is largest. However, no analogous studies have been performed to look for systematic effects of γ_{H_2} on formation of the first stars, where at least potentially the effects of variable γ_{H_2} are much larger. The few studies that do include non-constant γ_{H_2} (Silk 1983; Omukai & Nishi 1998; Abel et al. 2002; Yoshida et al. 2006; Ahn & Shapiro 2007; McKee & Tan 2008; Greif 2014; Stacy, Bromm & Lee 2016) have not systematically studied its effects, and have also included only variability due to vibrational degrees of freedom, not rotational ones. Our goal in this paper is to carry out a comprehensive study comparing a full quantum mechanical treatment of

the H_2 molecule to the classical approximation adopted in most earlier 3D simulations.

This paper is organized as follows. Section 2 discusses how we compute the adiabatic index of H_2 . Section 3 describes the simulation set-up and the physics included. Section 4 presents our results and findings. Finally, Section 5 summarizes our analysis.

2 ADIABATIC INDEX OF H_2

The adiabatic index of a gas partly composed of H_2 depends on the temperature, mass fraction of H_2 , and the ratio of ortho-to-para H_2 (which are the two nuclear spin orientations of the molecule, see Omukai & Nishi 1998; Glover & Abel 2008; Matthews, Petitpas & Aceves 2011). To calculate this dependence, we follow the approach of Krumholz (2014), though equivalent calculations may be found in Boley et al. (2007) and Tomida et al. (2013). Consider a gas containing multiple chemical species, each with mass fraction x_s , such that $\sum_s x_s = 1$. The relation between the net adiabatic index of all species and density is

$$\gamma_{\text{net}} = \frac{d \ln P}{d \ln \rho}, \quad (1)$$

where P is the pressure. ρ is the volume density, which is related to the number density (n_s) and mass fraction (x_s) as

$$n_s = \frac{x_s \rho}{A_s m}, \quad (2)$$

where m is one amu and A_s is the mass number of the species. The net adiabatic index for the system can be written as the ratio of specific heats at constant pressure and volume

$$\gamma_{\text{net}} = \frac{c_p/k_B}{c_v/k_B} = \frac{c_p/k_B + 1}{c_v/k_B}, \quad (3)$$

where c_p and c_v are the specific heats per H nucleon at constant volume and pressure, respectively. We obtain these from the internal energy per unit volume,

$$e_g = n_H k_B T \frac{d \ln z}{d \ln T}, \quad (4)$$

where z is the ensemble partition function given by the product of partition functions for the translational, rotational, and vibrational degrees of freedom $z = Z_{\text{trans}} Z_{\text{rot}} Z_{\text{vib}}$, T is the temperature, and n_H is the number density of H nuclei (which is invariant under chemical reactions). The specific heat per H nucleon at constant volume is related to e_g by

$$\frac{c_v}{k_B} = \frac{1}{n_H} \frac{\partial e_g}{\partial T}. \quad (5)$$

Using partition functions and mass fractions for ortho and para H_2 ($Z_{\text{rot}} = Z_{pH_2} Z_{oH_2}$, as defined below), this becomes

$$\begin{aligned} \frac{c_v}{k_B} = & \frac{3}{2} + x_{pH_2} \frac{\partial}{\partial T} \left(\frac{T^2}{Z_{pH_2}} \frac{\partial Z_{pH_2}}{\partial T} \right) + x_{oH_2} \frac{\partial}{\partial T} \left(\frac{T^2}{Z_{oH_2}} \frac{\partial Z_{oH_2}}{\partial T} \right) \\ & + (x_{oH_2} + x_{pH_2}) \frac{\theta_{\text{vib}}^2 \exp(-\theta_{\text{vib}}/T)}{T^2 [1 - \exp(-\theta_{\text{vib}}/T)]^2}, \end{aligned} \quad (6)$$

where $x_{H_2} = x_{oH_2} + x_{pH_2}$ and we have assumed that all species other than H_2 have no internal degrees of freedom. While an exact calculation of the partition function should also include contributions from electronic and nuclear degrees of freedom, these modes are not excited in the range of temperatures relevant to this study; hence, they can safely be ignored, and we can simply adopt $\gamma = 5/3$ for monoatomic species like He. Similarly, we ignore

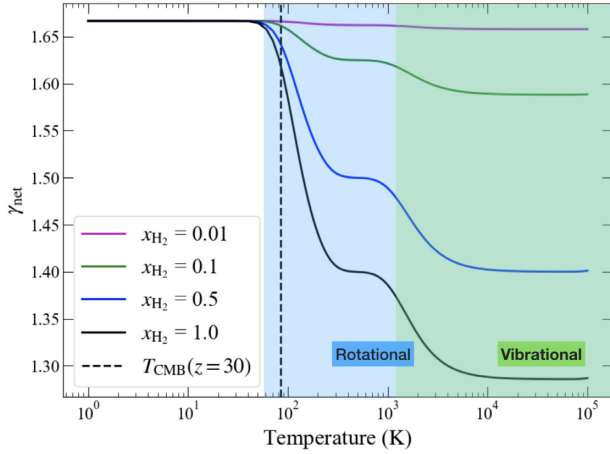


Figure 1. Net adiabatic index (γ_{net}) as a function of temperature for primordial gas with varying fractional abundances of H_2 , assuming an ortho-to-para ratio of 3:1 and no other species have any internal degrees of freedom. The dashed-black line marks the cosmic microwave background (CMB) floor at $z = 30$. The temperature range indicated in blue is dominated by the rotational degrees of freedom of H_2 whereas that in green is dominated by its vibrational degrees of freedom. The deviation of γ_{net} from the standard values is greatest for a completely molecular gas, and negligible if $x_{H_2} \lesssim 0.01$.

the effects of overlap between higher vibrational levels, vibrational continuum, and electronically excited levels of H_2 that occur at temperatures much higher than those we study in this work. We also use a fixed ortho-to-para ratio for reasons we discuss further below. The last term in equation (6) corresponds to vibrational degrees of freedom of H_2 , where $\theta_{\text{vib}} = 5987$ K (Draine, Roberge & Dalgarno 1983).

The rotational partition functions of para and ortho H_2 are given by

$$Z_{\text{pH}_2} = \sum_{J \text{ even}} (2J + 1) \exp \left[-\frac{J(J+1)\theta_{\text{rot}}}{T} \right], \quad (7)$$

$$Z_{\text{oH}_2} = e^{2\theta_{\text{rot}}/T} \left(\sum_{J \text{ odd}} 3(2J + 1) \exp \left[-\frac{J(J+1)\theta_{\text{rot}}}{T} \right] \right), \quad (8)$$

where $\theta_{\text{rot}} = 85.4$ K (Black & Bodenheimer 1975). The leading exponential term in the ortho H_2 partition functions ensures that rotation only contributes to internal energy when the rotational states are excited (Boley et al. 2007).

Fig. 1 shows the variation of the net adiabatic index of the system (γ_{net}) as a function of temperature (T) at different mass fractions of H_2 (x_{H_2}), assuming an ortho-to-para ratio of 3:1 (see below). When the gas is completely molecular (i.e. $\gamma_{H_2} = \gamma_{\text{net}}$), it can be described as monoatomic (three translational degrees of freedom) at low temperatures ($T < 50$ K) with $\gamma_{H_2} = 5/3$, and diatomic at high temperatures (three translational, two rotational, and two vibrational degrees of freedom) where the continuum limit is reached ($T \gtrsim 10^4$ K) with $\gamma_{H_2} = 9/7$.¹ Primordial star formation sits squarely in between these two regimes, where first the rotational modes are excited during collapse and then the vibrational modes are excited in accretion shocks around first stars, leading to the complex behaviour of γ_{H_2} as a function of T shown in Fig. 1.

¹Since H_2 is collisionally dissociated at temperatures well below 10 000 K, in reality it never reaches the high temperature continuum limit.

It should be noted that our calculation of the adiabatic index depends on our choice of the ratio of ortho- H_2 to para- H_2 , and any possible dependence of this ratio on temperature or density. However, Glover & Abel (2008) show that the ortho-to-para is not very sensitive to temperature at the redshifts important for Population III star formation, and the standard assumption of an ortho-to-para ratio of 3:1, i.e. $x_{\text{oH}_2} = 3x_{\text{pH}_2}$, as usually found in the present-day Universe (Sternberg & Neufeld 1999), produces results similar to a more detailed treatment. Due to interconversions facilitated by collisions with H^+ in the primordial gas, this ratio drops down to 0.25:1 at $z \approx 20$ in environments where the mass fraction of H_2 drops to 10^{-6} (Flower & Pineau des Forêts 2000; Flower & Harris 2007), but at such low H_2 abundances, the value of γ_{net} is essentially independent of γ_{H_2} in any event (Fig. 1). Keeping these studies in mind, we fix the ortho-to-para ratio to be 3:1 for our simulations.

3 NUMERICAL AND PHYSICAL INGREDIENTS

3.1 Numerical hydrodynamics

We use the adaptive mesh refinement (AMR; Berger & Colella 1989) code FLASH (Fryxell et al. 2000; Dubey et al. 2008). We utilize an approximate Riemann solver for our hydrodynamic simulations (Bouchut, Klingenberg & Waagan 2007, 2010) which was developed for FLASH by Waagan (2009) and Waagan, Federrath & Klingenberg (2011). We treat the self-gravity of the gas with a tree-based solver (Wünsch et al. 2018). We use the sink particle technique developed for FLASH (Federrath et al. 2010, 2011a, 2014) to follow the evolution of collapsing gas at high resolutions at late times. Sink particles are frequently used in hydrodynamic simulations of star formation as a proxy for stellar sources (Bate, Bonnell & Price 1995; Krumholz, McKee & Klein 2004; Jappsen et al. 2005; Wang et al. 2010; Padoan & Nordlund 2011; Gong & Ostriker 2013; Hubber, Walch & Whitworth 2013; Bleuler & Teyssier 2014; Jones & Bate 2018). These Lagrangian particles can travel inside the grid, accrete gas and contribute to the gravitational potential in the region. The sink particle method developed in Federrath et al. (2010) uses a rigorous set of checks to ensure that only Jeans unstable gas that is converging, bound and has a gravitational potential minimum in cells at the sink density threshold at the highest level of refinement is converted into a sink, thus avoiding artificial fragmentation. The density threshold where sink particles are created at the standard resolution used in our simulations (see below) is $1.45 \times 10^{-11} \text{ g cm}^{-3}$. We use the distribution of sink masses to study fragmentation around the primary sink. As the numerical scale we use in this work is much larger than the radii of actual protostars, we do not allow the merging of sink particles in our simulations (see, for e.g. Susa et al. 2014; Riaz et al. 2018).

In order to completely encompass the cloud that collapses to form stars, we define a cubical box of size $L = 2.4 \text{ pc}$ to run our simulations. We set the boundary conditions to be outflow-type to enable mass-loss from the cloud, if any, during star formation.² The boundary condition for gravity is ‘isolated’ (i.e. not periodic). We use a base grid of 8^3 cells plus 14 levels of refinement in this work, which results in a unit cell length at the highest level of refinement of $dx = 7.6 \text{ au}$ and a maximum resolvable density $n \sim 10^{15} \text{ cm}^{-3}$; the maximum effective resolution of the simulation

²Note that outflow in FLASH also means that inflow can occur.

is 65536³. This choice is motivated by optimizing the trade-off between higher resolution and computational costs. We repeat three representative simulations with different random seeds of turbulence (see Section 3.3) at 12, 13, 14, and 15 levels of refinement to check numerical convergence; we present the results of our convergence study in the Appendix and show that it is reasonable to believe convergence has been achieved to first order at resolution 14.

Numerous studies have shown that it is important to resolve the scales at which turbulence can amplify magnetic fields through the small-scale dynamo action (Sur et al. 2010; Federrath et al. 2010; Schleicher et al. 2010; Schober et al. 2012b; Brandenburg, Sokoloff & Subramanian 2012; Schober et al. 2012a; Bovino, Schleicher & Schober 2013a; Latif et al. 2013). The required resolution in this case is at least 30 cells per Jeans length (Federrath et al. 2011b), which is 7.5 times more than the Truelove criterion to avoid artificial collapse in gravitohydrodynamic simulations (Truelove et al. 1997). Although we do not include magnetic fields in this work, we satisfy the criterion suggested by Federrath et al. (2011b) by using 32 cells per Jeans length, to maintain self-consistency with other works (Sharda et al., in preparation). In fact, using less than 30 grid cells per Jeans length leads to underestimates not only of the amplification of magnetic fields, but also of the amount of kinetic energy that is resolved on the Jeans scale (Federrath et al. 2011b) and the structure of the gas (e.g. the scale height of accretion discs; see Federrath et al. 2014).

3.2 Primordial chemistry

We utilize the KROME package for primordial chemistry, which has been developed to include chemistry in hydrodynamic simulations for astrophysical applications (Grassi et al. 2014). KROME uses a subroutine of pre-designed and re-writable chemical networks for various astrophysical phenomena which can be embedded in numerical codes like FLASH. It uses the differential solver DLSODES (Hindmarsh 1980; Radhakrishnan & Hindmarsh 1993) to solve the reaction network and evolves the temperature and density of the system in accordance with the chemistry and the specified heating and cooling processes (Grassi et al. 2013; Bovino et al. 2013b). The network of primordial chemical reactions we use in our simulations is `react_primordial_3` which is the most robust primordial chemistry network and includes the following species: H, H₂, H⁺, H⁻, He, He⁺, He⁺⁺, H₂⁺, and e⁻.

We include a variety of chemical and radiative heating and cooling processes, all of which are computed by KROME. The cooling processes we include are (1) cooling by H₂ through excitation of ro-vibrational modes in H₂ and subsequent emission of photons, (2) cooling through collisionally induced emission (CIE) that occurs due to the formation of ‘supermolecules’ with finite electric dipole from collisions between different molecules, (3) cooling due to endothermic chemical reactions, (4) atomic cooling due to collisional ionization, collisional excitation, and recombination of primordial species and bremsstrahlung emission from ionized species, and (5) cooling due to Compton scattering of cosmic microwave photons by free electrons. In addition, we impose a constraint on the minimum temperature such that it never decreases beyond the cosmic microwave background (CMB) temperature at the assumed redshift [$T_{\text{CMB}}(z = 30) = 84.63$ K]. The heating processes we include are (1) chemical heating generated from reaction enthalpies and (2) compressional heating (as computed by the hydrodynamic module).

At high densities, the cooling rates are suppressed by opacity effects. For cooling due to H₂, we approximately account for

this by using the H₂ cooling function provided by Ripamonti & Abel (2004). This approximation diverges from the more detailed treatment of opacity by Hirano & Yoshida 2013 (see also Greif 2014; Hartwig et al. 2015) when $x_{\text{H}_2} \lesssim 0.5$. However, in practice these cooling functions differ only where the gas is dense enough to be optically thick, and has also been heated by adiabatic compression to the point where H₂ undergoes significant collisional dissociation. Such conditions prevail only at densities $\gtrsim 10^{16} \text{ cm}^{-3}$, an order of magnitude higher than those we resolve. Thus, over the density range we cover, the Ripamonti & Abel (2004) and Hirano & Yoshida (2013) H₂ cooling functions are very similar. Apart from this, the Ly α cooling formulation that we include in our simulations (in KROME) diverges from its true value in optically thick regimes where both the densities and temperatures are high; such regions constitute the accretion discs around sink particles, as we later show in Section 4. However, we do not expect this effect to significantly alter the temperature because the Ly α cooling rate is extraordinarily sensitive to temperature and only very weakly sensitive to optical depth (see e.g. section 2.1 of Ge & Wise 2017); thus, even fairly large optical depths alter the temperature relatively little. We also omit cooling due to H⁻. While this can be important in regions where H⁻ is abundant due to its large cross-section, the H⁻ abundance is very low at densities $\lesssim 10^{15} \text{ cm}^{-3}$ (Omukai 2001; Van Borm et al. 2014), the highest we resolve in this work.

Our chosen chemical network does not include deuterium, which was also produced by the big bang (Epstein, Lattimer & Schramm 1976). We choose to omit it because deuterium has no significant impact on the adiabatic index because of the low fractional abundance of HD as compared to H or H₂. HD can be an important coolant in low-density regions ($10^5 \leq n \leq 10^8 \text{ cm}^{-3}$) at temperatures of the order of 100 K (Galli & Palla 2002; Nagakura & Omukai 2005; Yoshida et al. 2007) in cases where the primordial gas does not go through an ionized phase (Johnson & Bromm 2006; Glover & Abel 2008). However, as we show below, our simulations start at $n \sim 10^4 \text{ cm}^{-3}$ and fragmentation occurs at densities that are 10^{4-5} times the density range quoted above. Similarly, we do not include primordial Li (Fields 2011), since it has been shown that its contribution to both chemistry and cooling is unimportant (Lepp & Shull 1984; Lepp, Stancil & Dalgarno 2002; Galli & Palla 2013; Liu & Bromm 2018).

3.3 Initial conditions

We initiate our simulations by setting up a spherical cloud core with a homogeneous density. Taking inspiration from cosmological simulations that form dark matter minihaloes where baryonic cores form in overdense regions, we begin from a core of mass $M_{\text{core}} = 1000 M_{\odot}$ and radius $R_{\text{core}} = 1 \text{ pc}$ (Abel, Bryan & Norman 2000; Abel et al. 2002; Bromm et al. 2002). These parameters are similar to that for Bonnor–Ebert spheres on the verge of collapse, and are often used in such simulations as initial conditions (e.g. Machida & Doi 2013; Hirano et al. 2014; Stacy & Bromm 2014; Susa et al. 2014; Hummel, Stacy & Bromm 2016; Riaz et al. 2018). Our initial density ($n_{\text{core}} = 9050 \text{ cm}^{-3}$) is thus in good agreement with the overdensity observed in such minihaloes in cosmological simulations. Based on 1D calculations of primordial cloud collapse using KROME that we run from low densities ($n = 1 \text{ cm}^{-3}$) and temperatures ($T = 100 \text{ K}$), we find that the temperature reaches 265 K by the time the density has reached $n \sim 10^4 \text{ cm}^{-3}$. Thus, we set $T_{\text{core}} = 265 \text{ K}$. This 1D model also sets the initial mass fractions of all species for our simulations. Specifically, we use $x_{\text{H}} = 0.7502$, $x_{\text{H}_2} = 0.0006$ and $x_{\text{He}} = 0.2492$, which also agree

Table 1. Initial conditions of the spherically homogeneous primordial cloud.

Parameter	Symbol	Value
Cloud mass	M_{core}	$1000 M_{\odot}$
Cloud radius	R_{core}	1 pc
Cloud number density	n_{core}	9050 cm^{-3}
Cloud temperature	T_{core}	265 K
Rotational/gravitational energy	$E_{\text{rot}}/E_{\text{grav}}$	0.03
Mass fraction of H	x_{H}	0.7502
Mass fraction of H_2	x_{H_2}	0.0006
Mass fraction of He	x_{He}	0.2492
CMB temperature at $z = 30$	T_{CMB}	84.63 K
Turbulence	v_{rms}	1.84 km s^{-1}
Sound speed	c_s	1.84 km s^{-1}

well with initial mass fractions for several other simulations at the same initial temperature and density; the He abundance is that predicted by the big bang nucleosynthesis (Steigman 2007; Galli & Palla 2013). To ensure the simulation box is in pressure equilibrium, we set the corresponding background density and temperature to be 100 times lower and higher, respectively. We put the initial core into solid body rotation around the \hat{z} -axis, with the initial angular velocity set such that the rotational energy is 3 per cent of the gravitational energy. This choice is motivated by the angular momentum of minihaloes observed in cosmological simulations (Bromm et al. 2002; Yoshida et al. 2006), and is roughly what is expected for a random turbulent field (Goodman et al. 1993; Burkert & Bodenheimer 2000; Lewis & Bate 2018).

Our initial velocity includes a random turbulent component on top of the organized rotational field. We only change the random seed value of turbulence between different runs. Our reasons for including turbulence are twofold: (1) cosmological simulations show that turbulence is driven in dark matter minihaloes by the motion of baryons towards the centre of the minihalo, leading to the formation of overdense regions ($n \sim 10^4 \text{ cm}^{-3}$) where collapse takes place (Greif et al. 2008; Prieto, Jimenez & Marti 2012; Cornuault et al. 2018); and (2) turbulence can also be generated by streaming velocities between the dark matter and baryons (Fialkov, Barkana & Visbal 2014) or primordial magnetic fields (Brandenburg, Enqvist & Olesen 1996; Kahnishvili, Brandenburg & Tevzadze 2016). Taking this into account and following Greif et al. (2008), we introduce rms velocity fluctuations (v_{rms}) equal to the sound speed (c_s) in the simulation box (i.e. we set an initially sonic turbulence with Mach 1; see also Clark et al. 2011b; Schober et al. 2012b; Riaz et al. 2018). The initial turbulent velocity field that we add has a power spectrum $P_v \sim k^{-1.8}$ from wavenumbers $k/(2\pi/L) = 2$ –20, where L is the side length of the computational domain. We choose the above scaling to model sonic turbulence that we include, which lies between the Kolmogorov turbulence ($k^{-1.67}$, for incompressible subsonic fluids) and Burgers turbulence (k^{-2} , for compressible supersonic fluids) and has been studied in detail in numerous works (e.g. Kritsuk et al. 2007; Federrath 2013). We summarize all properties of our initial conditions in Table 1.

4 RESULTS

We carry out two sets of simulations. One set uses a fixed value $\gamma_{H_2} = 7/5$, as is the common practice in first stars simulations; we refer to these runs as *Fixed* γ_{H_2} . The second set uses a value of γ_{H_2} computed via a full quantum mechanical treatment, as described in Section 2; we refer to these as the *Variable* γ_{H_2} simulations. We

carry out 40 realizations of each type of simulation, using different turbulent velocity fields. Velocity fields are matched in pairs of fixed and variable γ_{H_2} simulations, so the same 40 turbulent fields are used in each simulation set. We note that simulations with variable γ_{H_2} are not computationally expensive, and take the same time and resources as those with fixed γ_{H_2} . Thus, irrespective of the results, we highly recommend variable γ_{H_2} formulation be used for future studies of primordial star formation since it is more accurate. We define a sink formation efficiency

$$\text{SFE} = \frac{\sum M_{\text{sink}}}{M_{\text{core}}} \quad (9)$$

and present all analysis at SFE = 5 per cent. In other words, the analysis and figures we present is at the time when the sink particles have collectively accreted 5 per cent of the initial cloud mass. The reason for this is radiation feedback, which is not included in our simulations and can inhibit the growth of massive protostars $\gtrsim 25 M_{\odot}$ (Hosokawa et al. 2011; Schauer et al. 2015; Hosokawa et al. 2016). By limiting our analysis to the time when a relatively small mass has been accreted, we limit ourselves to considering the time before which our simulations will substantially deviate from reality.

4.1 Qualitative outcome

Fig. 2 shows the density-weighted projections of number density (through the \hat{z} -axis) in three representative runs from the fixed and variable γ_{H_2} cases where we find no (top panel), some (middle panel), and high fragmentation (bottom panel), respectively.³ The white dots marked with black boundaries in each panel represent the locations of sink particles in the corresponding runs. All the projections are focused on the 0.01 pc region around the most massive sink particle. While the runs with no fragmentation after the first sink is formed show a dense accretion disc around it, we detect diverse filamentary and spiral structures around the sink particles in other runs where subsequent fragmentation has occurred. The number densities we reach in the simulations are of the order of 10^{15} cm^{-3} where we begin to run into optically thick media. However, we expect the optically thick cooling rate approximation used from Ripamonti & Abel (2004) in KROME to remain accurate, because the densest regions that we resolve are almost fully molecular, as we notice from Fig. 3, which shows the mass fraction of H_2 in the same regions as illustrated in Fig. 2. However, where strong accretion shocks are present, H_2 has been dissociated into H. The presence of shocks can be seen through the velocity quivers overplotted on the pair of projection maps in the upper panel of Fig. 3 and the temperature field shown in Fig. 4. The temperature range has a strict lower limit given by the CMB temperature at our assumed redshift ($z = 30$, see Table 1) as well as a loose upper limit set by the onset of atomic cooling at temperatures greater than 10^4 K. The typical Mach numbers we find in the runs are between 2 and 35.

The qualitative outcome of our simulations, including the diversity in level of fragmentation, are similar to the results of other simulations of first star formation that include turbulence (Turk et al. 2012; Schober et al. 2012b; Riaz et al. 2018). Stars forming

³A movie showing the evolution of density and γ_{H_2} as collapse and fragmentation occur in a representative run is available as supplementary online material.

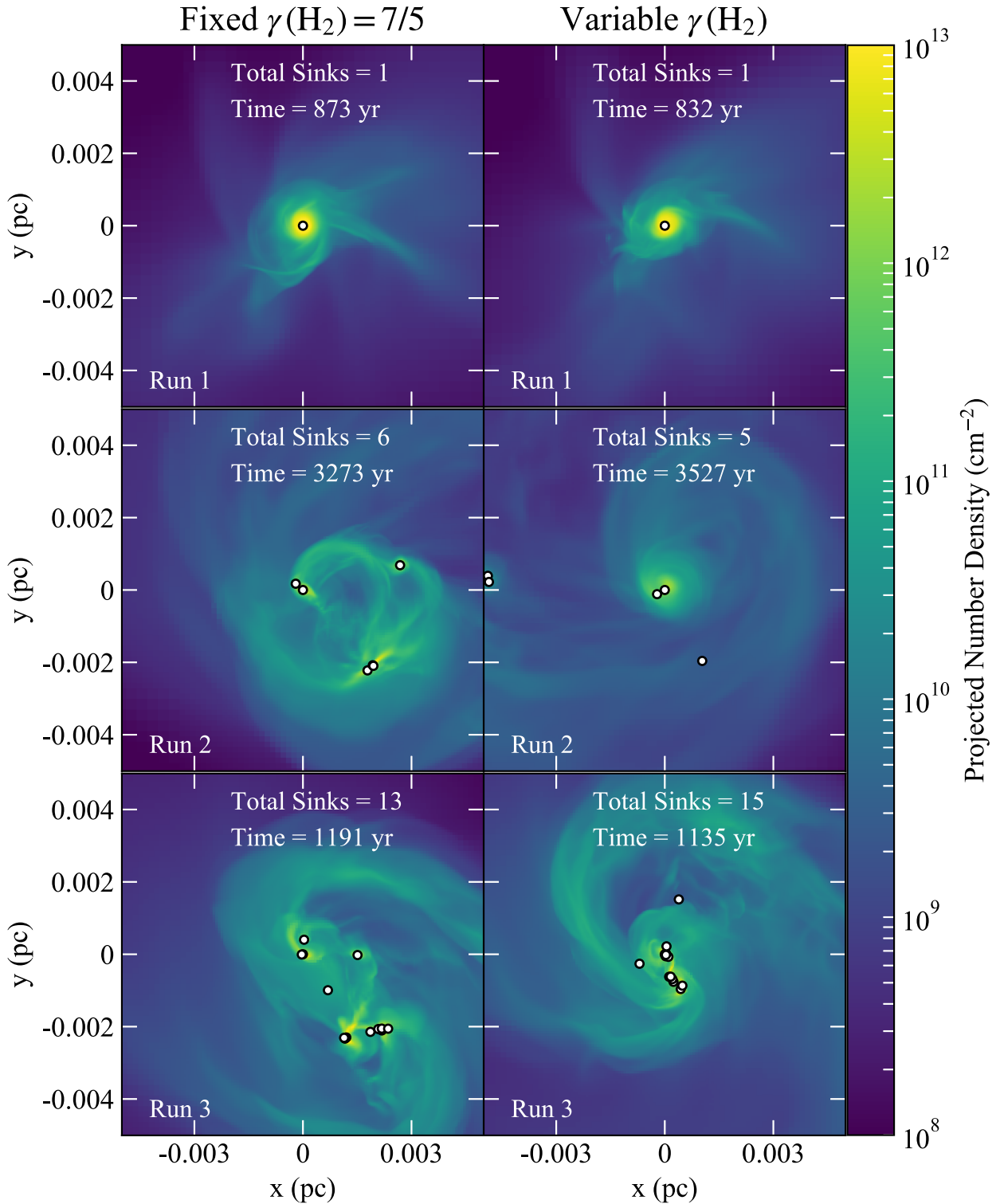


Figure 2. Face-on density-weighted projection maps of the number density (through the \hat{z} axis) for a pair of three representative runs showing no (*top panels*), some (*middle panels*), and high fragmentation (*bottom panels*) for fixed (left) and variable (right) γ_{H_2} , respectively. All the snapshots are taken when the sink(s) (shown in white circles with black boundaries) have collectively accreted 5 per cent of the initial cloud mass (SFE = 5 per cent, see equation 9). The snapshots cover a spherical region of radius 0.01 pc, centred on the most massive sink in the simulation. The time printed in each panel is the time since the formation of the first sink particle in each run. Each of the paired fixed and variable γ_{H_2} cases shown begins from identical initial conditions, so the differences seen in the corresponding maps arise solely due to variations in γ_{H_2} .

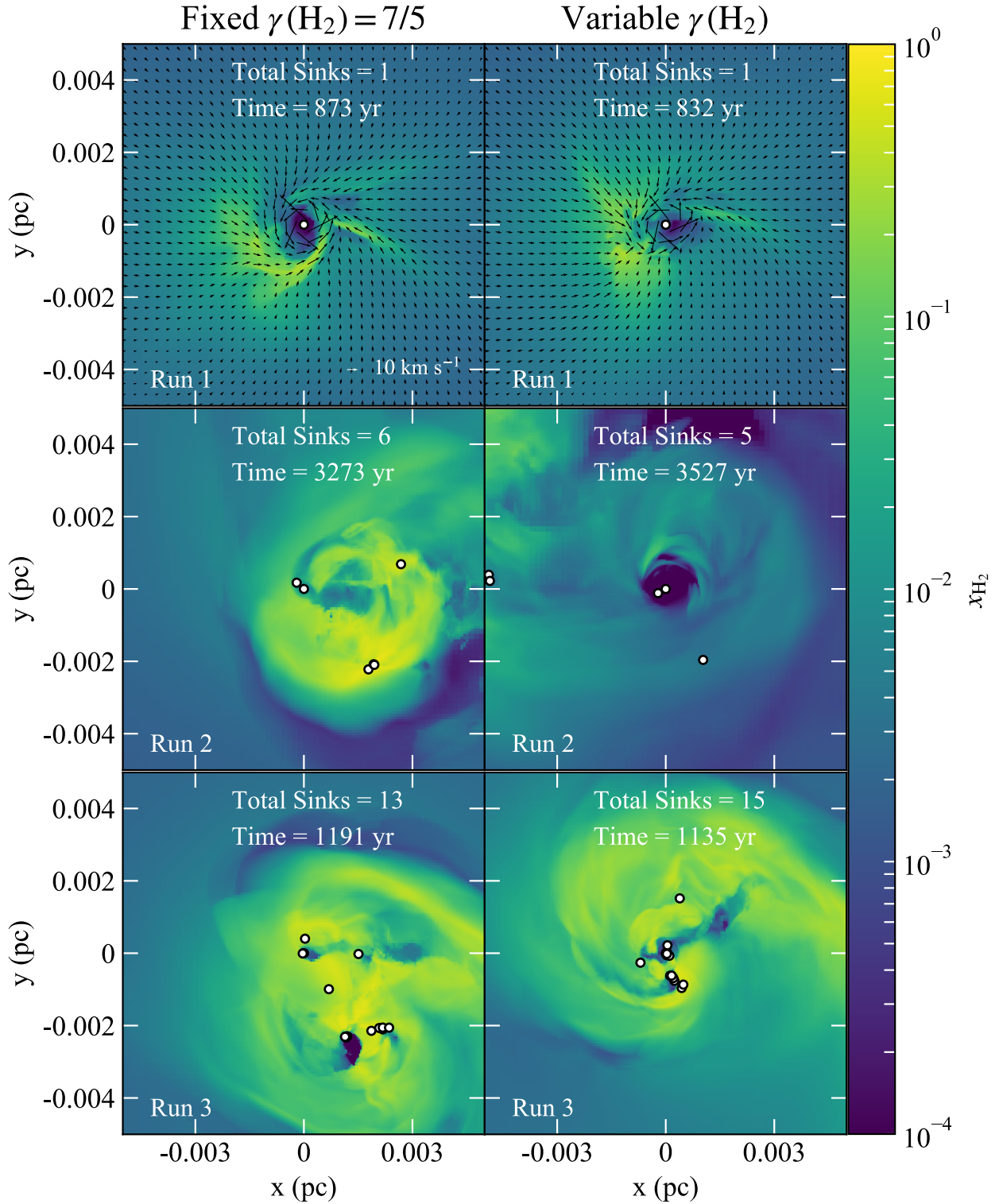


Figure 3. Same as Fig. 2 but showing the density-weighted mean mass fraction of H_2 (x_{H_2}). Quivers plotted on the top panels represent the velocity vectors.

in highly fragmented systems often experience fragmentation-induced starvation that limits the gas per star available for accretion (Kratter & Matzner 2006; Peters et al. 2010; Girichidis et al. 2012). This effect is more prominent for Population III star formation than for contemporary star formation, due to the smaller distances from the primary at which fragmentation occurs.

Fig. 5 shows the joint distributions of number density as a function of temperature, mass fraction of H_2 (x_{H_2}), adiabatic index of H_2 (γ_{H_2}), and the net adiabatic index of all species (γ_{net}) for a representative simulation of the variable γ_{H_2} case. We show these characteristics just before the formation of the first sink particle and at the end point of our simulations where SFE = 5 per cent.

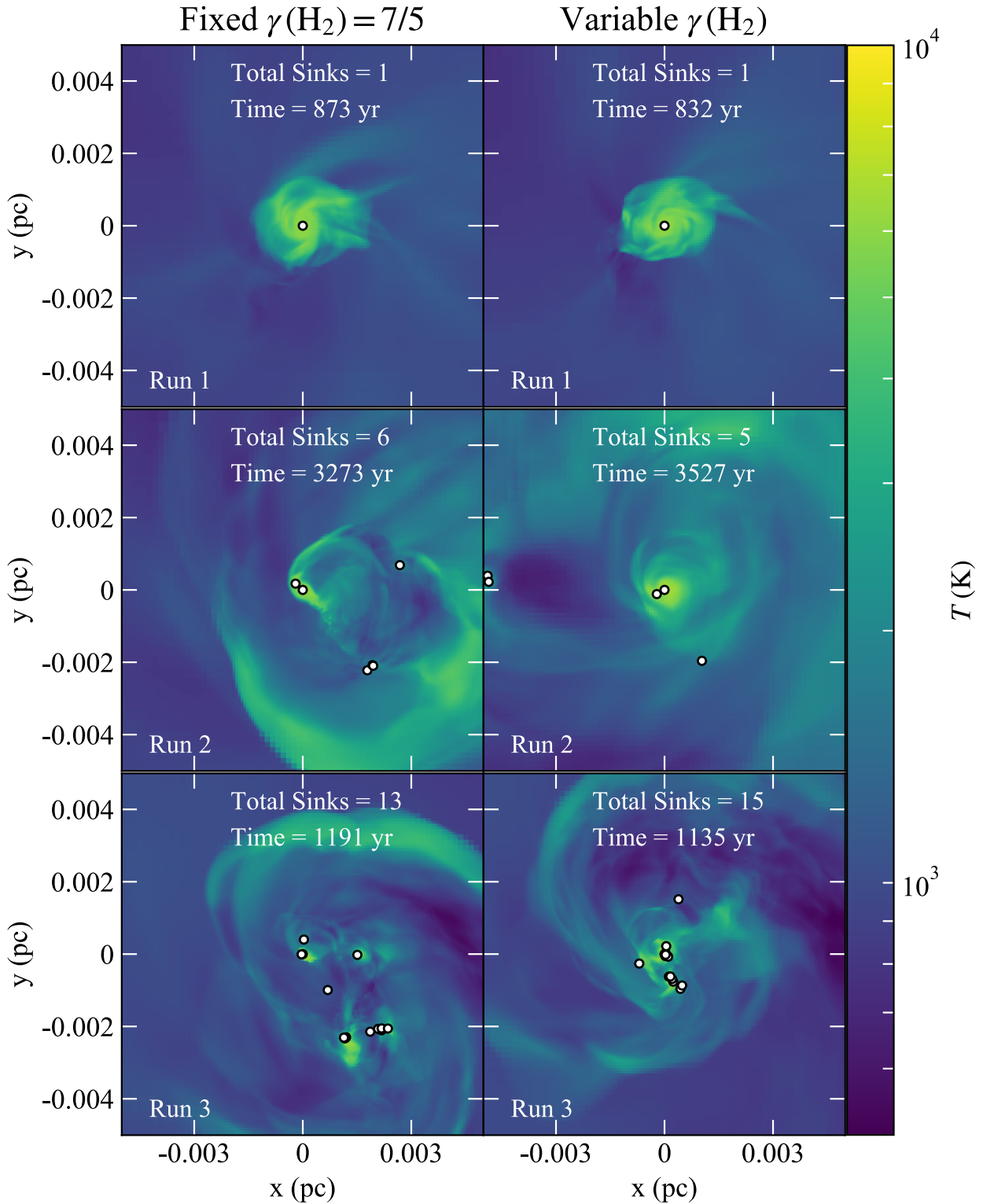


Figure 4. Same as Fig. 2 but showing the density-weighted mean temperature.

We sample these distributions over all the cells within 0.5 pc of the most massive sink in the simulation at SFE = 5 per cent. The evolution of temperature with density in the collapsing cloud closely follows the one zone model of Omukai et al. (2005), as can be noticed from the mean value of the $n - T$ distribution plotted as the black curve in the top panels of Fig. 5. For comparison, we

also plot the mean value of the corresponding fixed γ_{H_2} case in magenta. It is clear that the mean value between the two cases only slightly differs throughout the collapse of the cloud. The diverging behaviour from the mean at higher densities is due to the formation of accretion discs around sink particles that contain a huge diversity of cells with different positions in the $n - T$ space. There is a clear

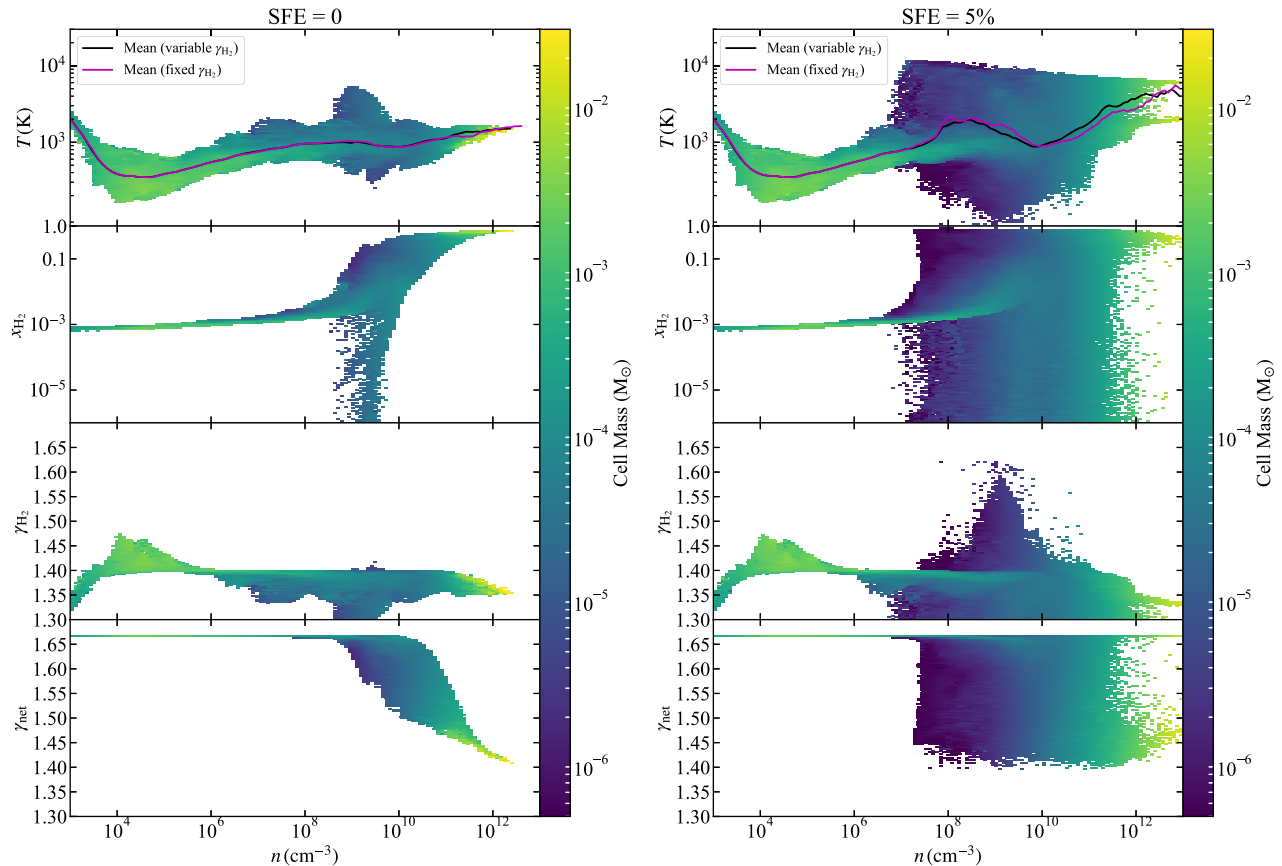


Figure 5. Joint distributions of number density (n) as a function of temperature (T , *first panel*), mass fraction of H_2 (x_{H_2} , *second panel*), adiabatic index of H_2 alone (γ_{H_2} , *third panel*) and of all gas (γ_{net} , *fourth panel*) in a spherical volume of radius 0.5 pc centred on the most massive sink particle. The two figures reflect the characteristics of the system just before the formation of the first sink and at SFE = 5 per cent. They belong to one of the 40 runs randomly selected from the variable γ_{H_2} subset. Also plotted in the top panels is the mean trend of T as a function of n for the variable (black) and the corresponding fixed γ_{H_2} (magenta) run.

scatter in the distributions that is a result of variations in temperature and mass fraction of H_2 , and the variance of the distribution of γ_{H_2} increases monotonically with time. The distributions have a number of features whose physical origin is easy to understand. At densities $n \lesssim 10^7 \text{ cm}^{-3}$, γ_{net} is very close to 5/3 because the H_2 fraction is tiny, as can be noticed from the second panel of Fig. 5. Only above this density does an appreciable H_2 fraction build up due to three-body reactions (Omukai et al. 2005; Glover & Abel 2008; Grassi et al. 2013); it also undergoes rapid dissociation due to high temperatures, thus leading to negligible x_{H_2} . At higher densities, the value of γ_{net} ranges from near 5/3 to near 7/5, tracking both H_2 fraction and temperature. The adiabatic index of the H_2 alone, γ_{H_2} , has a mean value of 1.39 with a standard deviation of 0.02, but there are excursions to both higher and lower values. Excursions to higher γ_{H_2} represent cells that have cooled to near the CMB floor of 85 K, cold enough for the rotational degrees of freedom to freeze out, while those to low γ_{H_2} are preferentially cells at temperatures of a few thousand K, where the vibrational degrees of freedom become excited and γ_{H_2} reaches an absolute minimum = $9/7 \approx 1.28$.

4.2 Mass distribution of sinks

We next examine the distribution of sink particle masses in the two sets of simulations. The fixed and variable γ_{H_2} cases form 186 and 192 sink particles in total, respectively. Fig. 6 shows the probability

distribution function (PDF) and cumulative distribution function (CDF) of the sink masses at the instant when 5 per cent of the total initial cloud mass has been accreted (i.e. SFE = 5 per cent), summed over all 80 simulations. We remind the reader that these are not the final masses, since we have not run to 100 per cent accretion, and do not include the feedback that would be required to do so. However, comparison of early fragmentation in the two simulation sets is none the less revealing of whether changes in the H_2 adiabatic index matter. We find that the mass distribution peaks around $1 M_\odot$ in both the fixed and variable γ_{H_2} cases, and rapidly declines for subsolar masses. Both the fixed and the variable γ_{H_2} cases have sink particles masses between 0.02 and $50 M_\odot$, with a mean of $10.5 M_\odot$. The two subsets further show quantitatively similar accretion rates of the different sink particles that form in the system. The apparent bi-modality in the distribution caused by the peak at $50 M_\odot$ is due to the fact that one-third of all the simulations only form a single massive star (no signs of fragmentation until SFE = 5 per cent). In such runs, the single sink particle accretes $50 M_\odot$.

To search for differences between the mass distributions for fixed and variable γ_{H_2} , we apply the Kolmogorov–Smirnov test (KS test), which yields a p -value of 0.28, implying that we cannot rule out the null hypothesis that the mass distribution is unaffected by our differing treatments of γ_{H_2} . Hence, even though the physical properties of the two cases are different (as discussed in Section 4.1), the mass distribution of the sink particles is statistically the same. Of course, we cannot rule out the possibility that a difference might

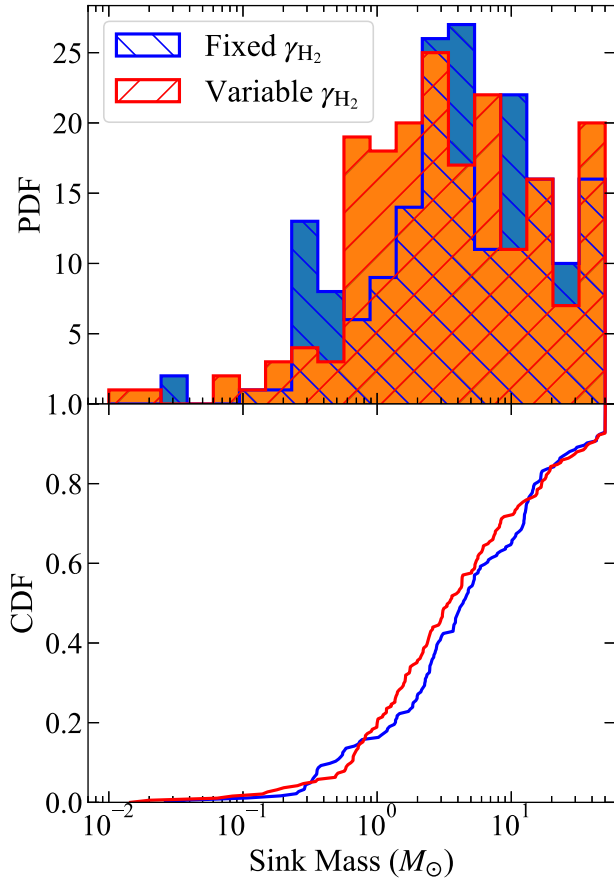


Figure 6. PDF (top panel) and CDF (bottom panel) of sink particle masses formed in all 80 simulations. The fixed γ_{H_2} case (blue) forms a total of 186 sink particles up to the point where 5 per cent of the initial cloud mass has been deposited in sink particles in each run (SFE = 5 per cent). The variable γ_{H_2} case (red) creates 192 sink particles. Comparing the two distributions with a KS test yields a p -value of 0.28, implying that we cannot rule out the null hypothesis that the two sets of sink particle masses were drawn from the same parent distribution. The peak at $50 M_\odot$ in the PDF and the corresponding jump in the CDF in both sets of runs is due to runs where no fragmentation occurs, and our condition of stopping at SFE = 5 per cent therefore results in a single sink particle of mass $50 M_\odot$.

become apparent if we performed a larger number of runs, or included feedback enabling the runs to continue further. However, at the level of data available (378 distinct sink particles, measured at SFE = 5 per cent), changing our treatment of γ_{H_2} has no detectable effect.

4.3 Multiplicity fraction

Given that our simulations frequently yield multiple stars (see Fig. 2), we next examine the multiplicity properties of the stars. A simulation that produces a realistic IMF of the first stars should also be able to explain or predict the fraction of Population III binaries or higher-order bound systems (Weidner, Kroupa & Maschberger 2009; Stacy, Greif & Bromm 2010), which is a crucial input to estimates of the rate of black hole or neutron star mergers, and similar high-energy phenomena.

We define multiplicity in our simulations following the algorithm of Bate (2009). In this algorithm, we recursively find the most

bound pair of sinks (i.e. sinks for which the sum of gravitational potential energy and kinetic energy around their common centre of mass is most negative) and replace them with a single sink at their center of mass, with mass equal to the sum of masses of the constituent sinks. The velocity of the replaced sink is then the velocity of the centre of mass of the constituent pair. Every iteration likewise finds the most bound pair in the system and replaces it with a single sink. This can lead to aggregation of sinks to higher orders, for example, when a sink that replaced two sinks in an earlier iteration now forms the most bound pair with a third sink. The exception to this rule is if aggregating the most bound pair would lead to a quintuple or higher system, which would almost certainly disintegrate dynamically were the simulation to be run long enough; if aggregating the most-bound pair would lead to such an outcome, we skip it and proceed to the next-most-bound pair that can be combined to produce an aggregate of <5 individual stars. The algorithm terminates if during any iteration there are no more bound pairs that can be aggregated to yield a combined system with multiplicity <5 .

The final result of this algorithm is that all sinks in each simulation are placed in multiplicity groups: isolated sinks that are not bound to any other sinks (S), bound pairs (B), triples (T), or quadruples (Q). Then, the multiplicity fraction is given as (e.g. Kouwenhoven et al. 2010; Bate 2012; Krumholz, Klein & McKee 2012)

$$mf = \frac{B + T + Q}{S + B + T + Q}. \quad (10)$$

This empirical definition has proven robust for use on observations because it does not change if the number of components in a bound system is updated (Hubber & Whitworth 2005), for example, if a system initially classified as a binary is later discovered to contain a third member.

Fig. 7 shows the CDF of mass for singles, binaries, triples, and quadruples in our simulations; note that the CDF we plot is the distribution of masses for *all* stars identified at a given multiplicity, not just for the primary in each system. The (fixed, variable) γ_{H_2} cases form (48, 53) single stars, (16, 24) binaries, (30, 15) triples, and (92, 100) quadruples, respectively. The mean value of multiplicity fraction (mf) we find for the fixed and variable γ_{H_2} cases is 0.45 and 0.37, respectively. Although the differences in the number of binaries and triples for the two cases is 33 and 100 per cent, respectively, we cannot classify them as significant because of the low number of such systems that form in our simulations. We compare the fixed and variable γ_{H_2} CDFs in each multiplicity bin using a KS test, obtaining p -values of 0.43, 0.17, 0.58, and 0.75, for singles, binaries, triples, and quadruples, respectively. As with the mass distribution for all stars, we detect no statistically significant difference between the fixed and variable γ_{H_2} runs for the singles, binaries, triples, and quadruples. We speculate that part of the reason that including variable γ_{H_2} has little effect is that a cancellation occurs: as shown in Fig. 1, depending on the density and temperature regime, γ_{H_2} can be both lower and higher than its classical value of 1.4. The former favours fragmentation (since a gas with lower γ is more compressible), while the latter opposes it, but since there are deviations to both lower and higher γ_{H_2} the effects roughly cancel out.

We can also compare the multiplicity fractions directly. Fig. 8 shows the CDF of the multiplicity fraction for the two cases. A KS test comparison of the two distributions yields a p -value of 0.72, indicating that the differences in multiplicity fraction are, like the differences in mass, not statistically significant. Fig. 9

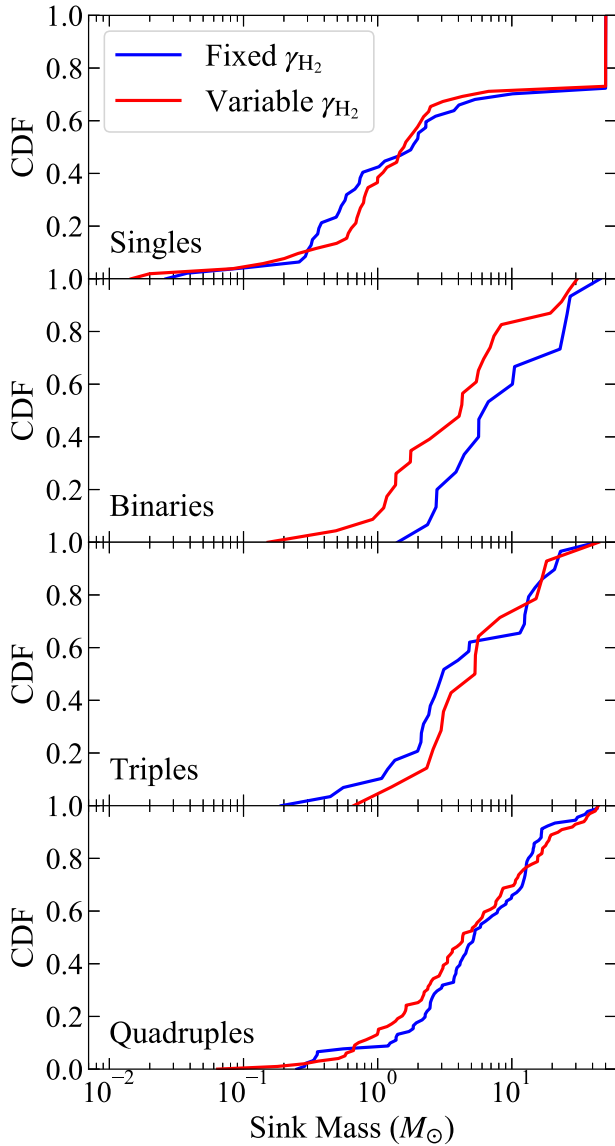


Figure 7. Cumulative mass distribution for stars classified as single, binary, triple, and quadruple (top to bottom) in the two cases of fixed and variable γ_{H_2} , at a time when 5 per cent of the initial cloud mass has been accreted by sink particles (SFE = 5 per cent). Stars are classified by multiplicity as described in the main text. The sudden vertical jump at $50 M_\odot$ in the case of single stars represents the runs that show no fragmentation until SFE = 5 per cent. Comparisons of the plotted mass distributions via KS tests yield p -values consistent with the null hypothesis that both runs are drawn from the same parent distribution.

shows the fraction of the mass in multiple systems that is in the primary (most massive star). Values close to unity indicate systems consisting of a dominant primary with small companions, and usually correspond to runs where fragmentation occurs only shortly before we reach SFE = 5 per cent, or to cases where fragments form earlier but are not able to accrete much mass. On the other hand, ratios farther from unity indicate more equal multiples, which generally result from near-simultaneous fragmentation at locations very close to each other, although there can be other possibilities. The p -value returned by a KS comparison of the variable and fixed γ_{H_2} distributions is 0.81, again revealing no statistically significant differences.

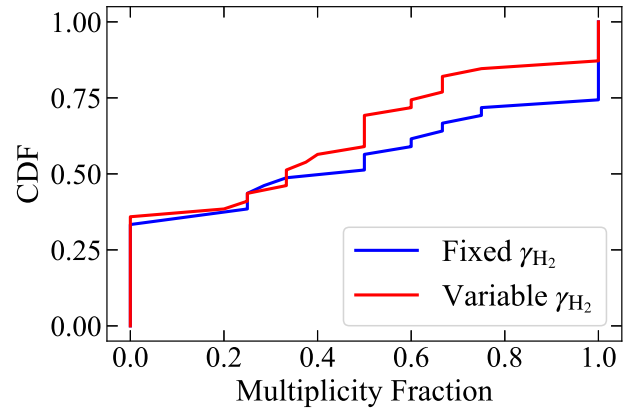


Figure 8. CDF of the multiplicity fraction (mf) sampled from 80 simulations for the fixed and variable γ_{H_2} cases, calculated using equation (10). The high fraction of mf at 0 multiplicity represents one-third of the total runs, where no fragmentation is observed. Similarly, runs where all the stars are bound (i.e. no singles) contribute to the jump seen at mf = 1. The KS test p -value for the two distributions of mf corresponding to the fixed and variable γ_{H_2} cases is 0.72.

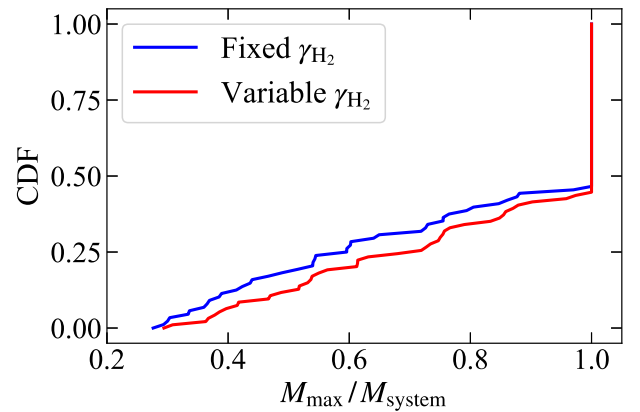


Figure 9. CDF of the ratio of the primary (most massive) star (M_{\max}) to the sum of masses of stars in a bound system (M_{system}) that can be a binary, triple, or quadruple. The substantial fraction of non-fragmented runs lead to this ratio being 1 with a high frequency.

5 CONCLUSIONS

In this work, we study the effects of the adiabatic index of molecular hydrogen (γ_{H_2}) on the fragmentation and mass distribution of the first protostars. H_2 is the primary component of the star-forming gas and the dominant cooling agent in zero metallicity primordial clouds where there is no dust. Thus, the thermodynamics are primarily controlled by H_2 and as such it is necessary to check whether the common approximation of treating H_2 as a classical diatomic gas with fixed adiabatic index $\gamma_{H_2} = 7/5$ is valid. The reason for concern is that, at the temperatures of a few hundred K found in primordial clouds and the accretion discs of the first stars, rotational and vibrational levels of H_2 are only starting to become excited, and thus H_2 behaves non-classically. Instead, its adiabatic index is a complex function of both temperature and the ratio of ortho-to-para H_2 .

We perform two sets of 3D simulations at high resolution (7.6 au) using the AMR hydrodynamic code FLASH. In the first

set, we fix $\gamma_{\text{H}_2} = 7/5$ and in the second we compute γ_{H_2} as a function of temperature and ortho-to-para ratio, using a full quantum mechanical treatment. We follow all simulations up to the time when 5 per cent of the initial cloud mass is accreted by sink particles, yielding a total of 378 sink particles from 80 simulations with different initial random turbulent velocity fields, with a mean sink particle mass of $10.5 M_{\odot}$. We show that primordial systems can undergo high fragmentation at distances as close as 5 au from the primary star, thus resulting in stars being bound to others soon after their formation; the mean multiplicity fraction is 0.4. However, around one-third of our simulations show no fragmentation even when the first star has accreted $50 M_{\odot}$. Hence, unless feedback effectively halts accretion on to the isolated massive stars, it seems likely that a great diversity of Population III stars existed, from single massive stars evolving in isolation to clustered formation of significantly less massive stars.

Comparing runs using identical initial conditions with fixed and variable γ_{H_2} reveals clear differences in physical properties such as density and temperature distributions, especially in regions where the net adiabatic index of all species (γ_{net}) is dominated by γ_{H_2} due to the high mass fraction of H_2 . We compare and analyse the mass distribution and multiplicity of the fixed and variable γ_{H_2} simulations; we find no statistically significant differences between the two. We also do not see any evidence of preferential formation of clustered systems in either of the two cases. Within the domains covered by this analysis, we therefore conclude that the standard approximation of molecular hydrogen as a classical diatomic gas during the formation of the first stars is valid, at least to first order during the first few thousand years after collapse of the formation of the first star. This may change with feedback, as feedback will alter the temperature distribution and hence the value of γ_{H_2} . Thus, it is possible that a full quantum mechanical treatment of the H_2 molecule will prove more important at later stages of the primordial star formation process. None the less, we recommend following the accurate treatment of the H_2 adiabatic index in future studies of formation of the first stars, because it is not computationally more expensive as compared to the classical treatment.

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SUPPORTING INFORMATION

Supplementary data are available at *MNRAS* online.

movie_gammah2.mpeg

movie_numdens.mp4

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APPENDIX A: CONVERGENCE STUDY

It is well known that hydrodynamic simulations of star and galaxy formation can be highly sensitive to the resolution or level of refinement that can be achieved (Commerçon et al. 2008; Meru &

Table A1. Summary of outcomes for three sets of variable γ_{H_2} runs (A, B, C) carried out at multiple resolutions (12, 13, 14, and 15) with different random turbulent fields. N_{sink} denotes the number of sink particles at SFE = 3.5 per cent and dx is the unit cell length at the highest level of refinement corresponding to the resolution used.

Property	Resolution	dx (au)	Run A	Run B	Run C
N_{sink}	12	30	2	4	2
	13	15	2	6	5
	14	7.6	3	6	13
	15	3.8	3	6	13

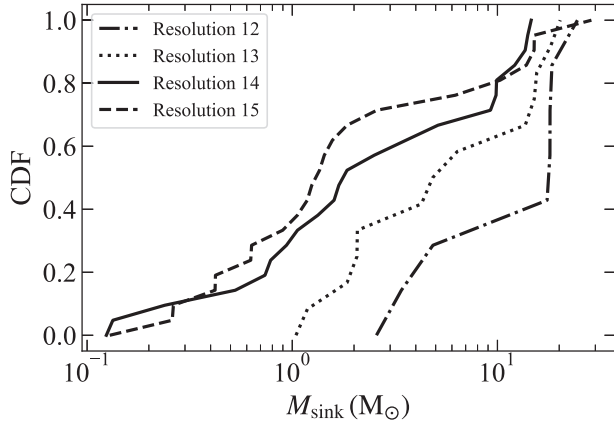


Figure A1. CDF of the sink particle mass accumulated over the three runs (A, B, C; see Table A1) at every resolution.

Bate 2011; Snaith et al. 2018). In the case of primordial star formation, the Jeans scale (and the fragmentation scale) depends on the resolution and thus plays a key role in setting the mass distribution of sink particles (Glover 2005; Stacy et al. 2010). Hence, it is necessary to check if the fragmentation we observe in our simulations is scale dependent. For this purpose, we repeat three runs with variable γ_{H_2} (to which we refer in this appendix as runs A, B, and C) from our total sample of 40 at four different resolutions with 12, 13, 14, and 15 levels of refinement, respectively (see Section 3.1 for a description of the levels of refinement). We select these three runs to represent cases of low, medium, and high fragmentation, respectively, at the resolution used in the main text (14 levels). To check for convergence, we compare the state of the runs at SFE = 3.5 per cent, rather than 5 per cent as in the main text. This is a pragmatic choice driven by the high computational cost of attempting to reach SFE = 5 per cent at the highest resolution. Table A1 shows the number of sinks formed, which remains unchanged between resolutions 14 and 15 for all the three runs, suggesting that our results are converged. We find further evidence of convergence at resolution 14 by plotting the CDF of the mass of sink particles accumulated from the three runs at every resolution, as we show in Fig. A1. In fact, the mean sink particle mass also remains the same at resolutions 14 and 15 in all the three runs. While the fragmentation pattern is not identical as we increase the resolution, we do not expect that it should be, since the flows are ultimately chaotic. These differences, however, do not appear to affect the first-order characteristics of primordial cloud collapse that we study in this work.

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