`VICE`: `Versatile Integrator for Chemical Evolution`

Science Documentation

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`VICE` is capable of simulating the enrichment of elements in galaxies that are produced in any part by core collapse supernovae, type Ia supernovae, and asymptotic giant branch stars. It does not model enrichment via the r-process in any way. It recognizes all 76 astrophysically produced elements on the periodic table from carbon to bismuth.

In this documentation we adopt the notation where $m = M/M_{\odot}$, a unitless mass measurement relative to the sun. We similarly note l and u as the lower and upper mass limits on star formation, respectively. Deviations from this notation will be made clear by the usage of a capital M, meant to denote a mass with dimensionality.

1) Background

1.1) Galactic Chemical Evolution

Big Bang Nucleosynthesis only produced hydrogen, helium, and trace amounts of lithium, the three lightest elements on the periodic table. Everything else is believed to have been produced by various channels of stellar evolution and supernovae, the yields of which are dictated by nuclear physics. This has an interesting implication for galaxies; being the sites of star formation and thus the production of heavy elements in the universe, their chemical patterns contain information that is almost if not entirely dependent on their formation and evolution through cosmic time. For more information and citations thereof, please see section 1 of Johnson & Weinberg (2019), MNRAS, XXXX, YYYY.

1.2) The Single-Zone Approximation

`VICE` operates under the single-zone approximation (sometimes also referred to as "box models", "one-zone models", or variations thereof). The fundamental assumption of these models is spatial homogeneity in all senses of the phrase. The single-zone approximation deliberately sacrifices all phase-space information; by assuming that gas, stars, heavy elements, and star formation efficiency is distributed uniformly, the need for N-body or hydro simulations is eliminated. This reduces the associated equations to a system of coupled integro-differential equations with time, which are easily integrated numerically. Mild numerical approximations often yield analytic results in some cases. This drastically reduces the computational expense associated with the single-zone approximation. For more information and citations thereof, please see sections 1 and 2 of Johnson & Weinberg, (2019), MNRAS, XXXX, YYYY. In this part of `VICE`'s documentation, we detail the analytic arguments behind the single-zone approximation and their numerical approximations implemented in `VICE`.

2.1) Stellar Lifetimes

We adopt in VICE the commonly used approximation for the lifetime of a star on the main sequence:

$$\tau_{\mathrm{MS}} \approx (10\ \mathrm{Gyr})m^{-3.5} \tag{1}$$

where 10 Gyr is the assumed lifetime of the sun on the main sequence. The scaling of $\tau_{\mathrm{MS}} \sim m^{-3.5}$ fails for high mass ($\gtrsim 8M_{\odot}$) stars, but these stars have lifetimes that are very short compared to the relevant timescales of galactic chemical evolution (~few Myr compared to ~few Gyr). In the manner that VICE is implemented, the lifetimes of extremely high mass stars are treated as instantaneous. This fails for low mass stars as well ($\lesssim 0.5M_{\odot}$), but these stars have such long lifetimes that none of them have evolved off of the main sequence over the entire lifetime of the universe.

By inverting this equation and solving for the mass and interpreting τ_{MS} as the age of the cluster t, we can solve for the turnoff mass $m_{\mathrm{to}}(t)$.

$$m_{\mathrm{to}}(t) = \left(\frac{t}{10\ \mathrm{Gyr}}\right)^{-1/3.5} \tag{2}$$

With the manner in which VICE is implemented, the turnoff mass is a much more numerically convenient quantity than the main sequence lifetimes of stars, because it is invoked in both the cumulative return fraction (section 2.2) and the main sequence mass fraction (section 2.3). Source code can be found at https://github.com/giganano/VICE/blob/master/vice/src/recycling.c.

2.2) The Cumulative Return Fraction

We define the cumulative return fration as the fraction of a single stellar population (or star cluster's) mass that is returned to the interstellar medium (ISM) as gas at the birth metallicity of the stars. As stars evolve off the main sequence, leaving behind a remnant, whatever mass does not end up in the remnant is returned to the ISM. This quantity varies with time and is thus denoted here accordingly as $r(t)$, where t is the star cluster's age. We demonstrate here that this quantity is uniquely specified the adopted initial mass function (IMF), the lifetimes of stars on the main sequence as a function of mass, and the mass of stellar remnants left behind also as a function of mass. It's full analytic expression is given by:

$$r(t) = \frac{\int_{m_{\text{to}}(t)}^{u} (m - m_{\text{rem}}) \frac{dN}{dm} dm}{\int_{l}^{u} m \frac{dN}{dm} dm} \tag{3}$$

The numerator is an integral over the stellar IMF from the *turnoff mass* m_{to} to the upper mass limit of star formation u weighted by the mass of these stars that does not end up in the remnant. The denominator is also an integral over the stellar IMF, but instead over the entire mass range for star formation l to u weighted by the initial mass of the stars m. This is nothing more than a mathematical statement of "ejected gas from dead stars over the sum total mass of all of them".

`VICE` adopts the model of Kalirai et al. (2008), ApJ, 676, 594, where the remnant mass is specified by:

$$M_{\text{rem}} = \begin{cases} 1.44 M_\odot & (M \geq 8 M_\odot) \\ 0.394 M_\odot + 0.109 M & (M < 8 M_\odot) \end{cases} \tag{4}$$

We derive the following expression given a power law IMF $dN/dm \propto m^{-\alpha}$ for the numerator of $r(t)$:

$$\int_{m_{\text{to}}}^{u} (m - m_{\text{rem}}) \frac{dN}{dm} dm = \frac{\beta}{2-\alpha} m^{2-\alpha} \Big|_{m_{\text{to}}(t)}^{u} - \begin{cases} \frac{1.44}{1-\alpha} m^{1-\alpha} \Big|_{m_{\text{to}}(t)}^{u} & (m_{\text{to}}(t) \geq 8) \\ \frac{1.44}{1-\alpha} m^{1-\alpha} \Big|_{8}^{u} + \left[\frac{0.394}{1-\alpha} m^{1-\alpha} + \frac{0.109}{2-\alpha} m^{2-\alpha} \right]_{m_{\text{to}}(t)}^{8} & (m_{\text{to}}(t) < 8) \end{cases} \tag{5}$$

This solution is analytic, and thus without any numerical approximations. For piecewise IMFs, this becomes a summation over the relevant mass ranges of the IMF where each term has the exact same form. The normalization of the IMF is irrelevant, because the same normalization appears in the denominator, and they thus cancel.

Also for a power law IMF with index α, we derive the following expression for the denominator of $r(t)$:

$$\int_{l}^{u} m \frac{dN}{dm} dm = \frac{1}{2-\alpha} m^{2-\alpha} \Big|_{l}^{u} \tag{6}$$

Weinberg, Andrews & Freudenburg (2017), ApJ, 837, 183 adopted instantaneous recycling, whereby a given fraction of a single stellar population's mass is returned to the ISM at the same metallicity instananeously. They demonstrated that $r_{\text{inst}} = 0.2$ and $r_{\text{inst}} = 0.4$ are good approximations for the Salpeter[1] and Kroupa[2] IMFs. This reduces the more sophisticated formulation detailed here to

$$r(t) \approx \begin{cases} r_{\text{inst}} & (t = 0) \\ 0 & (t \neq 0) \end{cases} \tag{7}$$

`VICE` gives users the ability to specify an instantaneous recycling parameter, but implements continuous recycling by default. These are the mathematical expressions implemented in `VICE`. Source code can be found at `https://github.com/giganano/VICE/blob/master/vice/src/recycling.c`.

We plot $r(t)$ as a function of time for both Kroupa and Salpeter IMFs in figure 1. The offset between the two IMFs is due to the difference in the number of low mass stars as predicted by the two IMFs.

[1] Salpeter (1955), ApJ, 121, 161
[2] Kroupa (2001), MNRAS, 322, 231

2.3) The Main Sequence Mass Fraction

We define the main sequence mass fraction as the fraction of a single stellar population's mass that is still in the form of main sequence stars. We denote this quantity as $h(t)$[3], where t is the star cluster's age. We demonstrate that this quantity is uniquely specified by the adopted stellar initial mass function (IMF) and the lifetimes of stars on the main sequence. It's analytic expression is given by:

$$h(t) = \frac{\int_l^{m_{\text{to}}(t)} m\frac{dN}{dm}dm}{\int_l^u m\frac{dN}{dm}dm} \tag{8}$$

Both the numerator and the denominator are mass-weighted integrals over the IMF, but the numerator does not count evolved stars. This is purely a mathematical statement of "main sequence mass over initial mass."

For a power law IMF $dN/dm \propto m^{-\alpha}$,

$$h(t) = \frac{\frac{1}{2-\alpha}m^{2-\alpha}\Big|_l^{m_{\text{to}}(t)}}{\frac{1}{2-\alpha}m^{2-\alpha}\Big|_l^u} \tag{9}$$

It may be tempting to cancel the factor of $1/2 - \alpha$, but much more careful considerations must be taken for piece-wise IMFs like Kroupa[4].

$$h(t) \rightarrow \frac{\left[\sum_i \frac{1}{2-\alpha_i}m^{2-\alpha_i}\right]_l^{m_{\text{to}}(t)}}{\left[\sum_i \frac{1}{2-\alpha_i}m^{2-\alpha_i}\right]_l^u} \tag{10}$$

where the summation is over the relevant piece-wise mass ranges.

`VICE` currently onlow allows functionality for the Kroupa and Salpeter[5] IMFs. In the case of the Kroupa IMF, α = 0.3 [1.3] [2.3] for stellar masses in the range $\leq 0.08M_\odot$ [$0.08M_\odot \leq M \leq 0.5M_\odot$] [$\geq 0.5M_\odot$]. For Salpeter, $\alpha = 2.35$ for all stellar masses.

`VICE` implements the main sequence mass fraction self-consistently given the user's specified stellar IMF. Source code can be found at `https://github.com/giganano/VICE/blob/master/vice/src/recycling.c`.

We plot $h(t)$ in the right-hand panel of Figure 1 for both Kroupa and Salpeter initial mass functions. The offset between the two is due to the difference in the number of low mass stars as predicted by the two IMFs. As discussed in section x.x, $h(t) \approx 1 - r(t)$ fails at the $\sim$15% level for single stellar populations. For this reason, the recycling fraction is not used in determing the rate of enrichment from AGB stars.

[3] h rather than m since m already denotes mass. We choose h for hydrogen fusion in the cores of these stars.
[4] Kroupa (2001), MNRAS, 322, 231
[5] Salpeter (1955), ApJ, 121, 161

2.4) Enrichment from Single Stellar Populations

While galaxies form stars continuously, sometimes astronomers are interested in the enrichment patterns of individual stellar populations. This is inherently cheaper computationally, since this is only one stellar population while a galaxy simulation would take into account multiple stellar populations.

`VICE` includes functionality for simulating the mass production of a given element from a single stellar population (i.e. an individual star cluster) of given mass and metallicity under the adopted yields. This by construction does not take into account depletion from infalling low metallicity gas and star formation, ejection in outflows, recycling, etc. It only calculates the mass of the element produced as a function of time.

At time $t = 0$, there is no mass produced, because this is adopted as the time at which the star cluster forms. Because `VICE` operates under the assumption that all core-collapse supernovae happen instantaneously, at $t = \Delta t$, the entire core-collapse nucleosynthetic yield is injected:

$$\Delta M_x = y_x^{\text{CC}}(Z)M_* \tag{11}$$

where $y_x^{\text{CC}}(Z)$ is the user's current yield setting for core collapse supernovae at the metallicity of the stars Z. At subsequent timesteps, enrichment from asymptotic giant branch stars:

$$\dot{M}_x^{\text{AGB}}\Delta t \approx y_x^{\text{AGB}}(m_{\text{to}}(t)|Z)M_*[h(t) - h(t + \Delta t)] \tag{12}$$

and type Ia supernovae:

$$\dot{M}_x^{\text{Ia}}\Delta t \approx y_x^{\text{Ia}}M_* \frac{R_{\text{Ia}}(t)}{\int_0^\infty R_{\text{Ia}}(t')dt'} \tag{13}$$

are injected. For details on these equations, see sections 4.3 (SNe Ia) and 4.4 (AGB stars). These are the same equations that are implemented in simulating enrichment under the single-zone approximation, but applied to only one episode of star formation.

Users can run these simulations directly by calling `vice.single_stellar_population`. Python wrapping for this function can be found at `https://github.com/giganano/VICE/blob/master/vice/core/_wrapper.pyx`, with source code at `https://github.com/giganano/VICE/blob/master/vice/src/metals.c`.

3.1) Inflows, Star Formation, and Efficiency

For a spatially homogeneous cloud of gas with mass infall rate (IFR) $\dot{M}_{\text{in}}$, star formation rate (SFR) $\dot{M}_*$, and outflow rate (OFR) $\dot{M}_{\text{out}}$, the time-derivative of the mass of the ISM gas is given by:

$$\dot{M}_{\text{g}} = \dot{M}_{\text{in}} - \dot{M}_* - \dot{M}_{\text{out}} + \dot{M}_{\text{r}} \tag{14}$$

where $\dot{M}_{\text{r}}$ is the rate of recycling from stars evolving off of the main sequence and returning gas to the ISM at their birth metallicity. Equation 14 is approximated numerically in the following manner:

$$\Delta M_{\text{g}} \approx \dot{M}_{\text{g}}\Delta t = \dot{M}_{\text{in}}\Delta t - \dot{M}_*\Delta t - \dot{M}_{\text{out}}\Delta t + \dot{M}_{\text{r}}\Delta t \tag{15}$$

As it turns out, it is numerically easier to determine the total mass recycled in a given time interval than it is to determine its time derivative. Since this is directly the quantity of interest, there is no need to complicate things further. See section 3.x for details.

By construction, `VICE` operates such that the user specifies either an infall history ($\dot{M}_{\text{in}}$ as a function of time), a star formation history ($\dot{M}_*$ as a function of time), or the gas history (M_{g} as a function of time). The user also specifies a star formation efficiency prescription:

$$\tau_* \equiv M_{\text{g}}/\dot{M}_* \tag{16}$$

τ_* can be any arbitrary function of time that the user has coded into `python`, allowing simulation of star formation efficiency prescriptions of arbtirary complexity. With, one of either $\dot{M}_{\text{in}}$, $\dot{M}_*$, or M_{g} specified by the user, τ_*, and the implementation of $\dot{M}_{\text{out}}$ and $\dot{M}_{\text{r}}$ detailed in this section, the solution to equation 14 is unique.

This is how the evolution of the gas supply is implemented in `VICE`. Source code can be found at https://github.com/giganano/VICE/blob/master/vice/src/metals.c.

3.2) Gas Outflows

Most galactic chemical evolution models adopt a dimensionless parameter known as the *mass loading factor*, which quantifies the strength of galactic winds as the ratio of the outflow rate to the star formation rate $\eta \equiv \dot{M}_\text{out}/\dot{M}_*$. In Johnson & Weinberg (2019), we introduced a new parameter into single-zone galactic chemical evolution modeling in an attempt to generalize this relationship, which we dubbed the *smoothing time*. This is the timescale on which the star-formation rate is averaged (or "smoothed") to determine the outflow rate:

$$\begin{aligned}\dot{M}_\text{out} &= \eta(t)\langle\dot{M}_*\rangle_{\tau_\text{s}} \\ &= \begin{cases} \frac{\eta(t)}{\tau_\text{s}}\int_{t-\tau_\text{s}}^{t}\dot{M}_*(t')dt' & (t \geq \tau_\text{s}) \\ \frac{\eta(t)}{t}\int_{0}^{t}\dot{M}_*(t')dt' & (0 \leq t \leq \tau_\text{s}) \end{cases}\end{aligned} \tag{17}$$

Under this formulation, the expression is piece-wise to ensure no numerical artifacts are introduced by smoothing over the star formation history evaluated from a negative timestep. `VICE` implements the following numerical approximation:

$$\dot{M}_\text{out} = \begin{cases} \eta(t)\frac{\Delta t}{\tau_\text{s}}\sum_{i=0}^{\tau_\text{s}/\Delta t}\dot{M}_*(t - i\Delta t) & (t \geq \tau_\text{s}) \\ \eta(t)\frac{\Delta t}{t}\sum_{i=0}^{t/\Delta t}\dot{M}_*(t - i\Delta t) & (0 \leq t \leq \tau_\text{s}) \end{cases} \tag{18}$$

In words, at each timestep `VICE` simply looks back the number of timesteps corresponding to the smoothing time, and determines the arithmetic mean of the star formation rate over those timesteps. An advantage of this formulation is that when $\tau_\text{s} < \Delta t$, `VICE` numerically recovers the traditional relation $\dot{M}_\text{out} = \eta(t)\dot{M}_*(t)$ automatically.

The mass loading parameter is a user-specified function of time. By implementing $\eta(t)$ in this manner, `VICE` achieves the capability of simulation galaxies with arbitrarily complex mass loading factors. We clarify that it is only the star formation rate which is time-averaged under this formulation; the user-specified $\eta(t)$ is taken to be an instantaneous function.

Source code can be found at `https://github.com/giganano/VICE/blob/master/vice/src/metals.c`.

3.3) Recycling

As stars evolve off of the main sequence, the mass that does not end up in the remnant is returned to the interstellar medium. The net effect of this from all previous episodes of star formation quantifies the rate of mass recycling.

$$\dot{M}_\text{r} = \int_0^t \dot{M}_*(t - t')\frac{dr(t')}{dt}dt \tag{19}$$

Obtaining the cumulative return fraction itself is somewhat more feasible than its time derivative. Since this is truly the quantity of interest anyway, we approximate the total mass recycled in a given timestep in the following manner.

$$\Delta M_\text{r} \approx \dot{M}_\text{r}\Delta t = \sum_{i=0}^{t/\Delta t} \dot{M}_*(t - i\Delta t)[r((i+1)\Delta t) - r(i\Delta t)]\Delta t \tag{20}$$

Since $r(t)$ is calculated numerically in each `VICE` integration, it is easier and thus faster computationally to determine the total mass recycled in a given timestep rather than the time-derivative $\dot{M}_\text{r}$.

`VICE` also allows users to pass an instantaneous recycling parameter r_inst, in which case the recycled mass is simply:

$$\dot{M}_\text{r}\Delta t \approx r_\text{inst}\dot{M}_* \tag{21}$$

Weinberg, Andrews & Freudenburg (2017), ApJ, 837, 183 found that this is a good approximation, with $r_\text{inst} \approx 0.4(0.2)$ for a Kroupa (Salpeter) IMF as recommended values.

This is how recycling is implemented numerically in `VICE`. By default, it will adopt the continuous recycling prescription of equation 20. Source code can be found at `https://github.com/giganano/VICE/blob/master/vice/src/recycling.c`.

4.1) The Enrichment Equation

For an arbitrary element x on the periodic table, the enrichment equation has the following general form:

$$\dot{M}_x = \dot{M}_x^{\text{CC}} + \dot{M}_x^{\text{Ia}} + \dot{M}_x^{\text{AGB}} - \frac{M_x}{M_{\text{g}}}[\dot{M}_* + \xi_{\text{enh}}\dot{M}_{\text{out}}] + \dot{M}_x^{\text{r}} + Z_{\text{x,in}}\dot{M}_{\text{in}} \tag{22}$$

This equation is nothing than a mathematical statement that at any given time (from left to right on the right-hand side), the element x is enriched via core-collapse supernovae (CCSNe), type Ia supernovae (SNe Ia), and asymptotic giant branch (AGB) stars, while simultaneous being depleted due to star formation at the current metallicity of the interstellar medium (ISM) M_x/M_{g} and outflows at some multiplicative factor ξ_{enh} above the ISM metallicity, re-enriched due to the recycling from previous generations of stars, and inflows of some metallicity $Z_{\text{x,in}}$.

We detail the $\dot{M}_x^{\text{CC}}$, $\dot{M}_x^{\text{Ia}}$, and $\dot{M}_x^{\text{AGB}}$ term individually, and the rest of them here. Source code for the implementation of this equation in `VICE` can be found at https://github.com/giganano/VICE/blob/master/vice/src/metals.c.

`VICE` operates under the assumption that star formation occurs at the current metallicity of the ISM M_x/M_{g}. Hence the $-(M_x/M_{\text{g}})\dot{M}_*$ sink term in the enrichment equation.

Many galactic chemical evolution models have operated under the assumption that outflows occur at or near the meatllicity of the ISM (i.e. $\dot{M}_x^{\text{out}} \approx (M_x/M_{\text{g}})\dot{M}_{\text{out}}$). However, recent work in the literature from both simulations and observations have suggested that this may not be the case. Therefore, `VICE` allows outflows to occur at some multiplicative factor of the ISM metallicity, which may vary with time. Hence the $(M_x/M_{\text{g}})\xi_{\text{enh}}\dot{M}_{\text{out}}$ sink term in the enrichment equation.

At any given time, there will be nonzero metallicity stars returning gas to the ISM at their birth metallicity. This is simply similar to the rate of gas recycling as discussed in section 3.3, but weighted by the metallicities of the stars. Since `VICE` operates under the assumption that star formation occurs at the metallicity of the ISM:

$$\begin{aligned} \dot{M}_x^{\text{r}} &= \int_0^t \dot{M}_*(t-t')Z_x^{\text{ISM}}(t-t')\frac{dr(t')}{dt}dt \\ \dot{M}_x^{\text{r}}\Delta t &\approx \sum_{i=0}^{t/\Delta t} \dot{M}_*(t-i\Delta t)Z_x^{\text{ISM}}(t-i\Delta t)[r((i+1)\Delta t) - r(i\Delta t)]\Delta t \end{aligned} \tag{23}$$

In the event that the user has specified instantaneous recycling, this equation simplifies:

$$\dot{M}_x^{\text{r}}\Delta t \approx r_{\text{inst}}\dot{M}_* Z_x^{\text{ISM}}\Delta t \tag{24}$$

This is the recycling rate as it is implemented in `VICE`. Source code can be found at https://github.com/giganano/VICE/blob/master/vice/src/recycling.c.

At any given timestep, there is gas infall onto galaxies of a given metallicity Z. This introduces a $Z_{\text{x,in}}\dot{M}_{\text{in}}$ term into the enrichment equation quantifying the addition of a given element x due to metal-rich infall. `VICE` allows users to specify a function of time $Z_{\text{x,in}}$ for each individual element. In this manner, `VICE` supports simulations of metal-rich infall with full generality.

4.2) Core Collapse Supernovae

Core collapse supernovae (CCSNe) are the explosions of massive stars ($\gtrsim 8M_\odot$) at the end of the nuclear lifetimes. Due to the steep nature of the lifetime-stellar mass relationship, these stars have lifetimes that are extremely short compared to the relevant timescales of galactic chemical evolution (~few Myr compared to ~few Gyr). This means that, to an extremely good approximation, the lifetimes of these stars can be treated as instantaneous in galactic chemical evolution models. The enrichment from CCSNe thus instantaneously converts some fraction of a single stellar population's mass into a given element x under this approximation, implying a linear relationship between the rate of mass enrichment and the star formation rate:

$$\dot{M}_x^{\text{CC}} = y_x^{\text{CC}}(Z)\dot{M}_* \tag{25}$$

where $y_x^{\text{CC}}(Z)$ is the fraction of the stellar population's mass which is converted to the element x, which may be dependent on the metallicity Z. This is the IMF-integrated fractional nucleosynthetic yield of the element x from CCSNe; see section x.x for more information on this quantity.

Source code for the implementation of this equation in `VICE` can be found at https://github.com/giganano/VICE/blob/master/vice/src/ccsne.c.

4.3) Type Ia Supernovae

Type Ia supernovae (SNe Ia) are the thermonuclear detonations of white dwarf (WD) stars. Being the remnants of lower mass stars, WDs are produced on longer timescales than CCSNe; this requires an intrinsic delay-time distribution (DTD) R_{Ia} to accurately model this channel of enrichment.

We define the SNe Ia DTD as the rate of SNe Ia explosions associated with only stellar population. A time t following the formation of a single stellar population, the rate of enrichment of an element x is given by the normalized rate of SNe Ia:

$$\dot{M}_x^{\text{Ia}} = y_x^{\text{Ia}} M_* \frac{R_{\text{Ia}}(t)}{\int_0^\infty R_{\text{Ia}}(t')dt'} \tag{26}$$

`VICE` allows users to specify any arbitrary function of time as $R_{\text{Ia}}(t)$. It also has built-in functionality for exponential DTDs ($R_{\text{Ia}} \propto e^{-t/\tau_{\text{Ia}}}$ for some τ_{Ia}) as well as power-law DTDs with index 1.1 ($R_{\text{Ia}} \propto t^{-1.1}$). In all cases, the normalization of the DTD is taken care of automatically:

$$\begin{aligned} R_{\text{Ia,reduced}}(t) &= \frac{R_{\text{Ia}}(t)}{\int_0^\infty R_{\text{Ia}}(t')dt'} \\ &\rightarrow \begin{cases} 0 & (0 \leq t \leq t_{\text{D}}) \\ \dfrac{R_{\text{Ia}}(t)}{\sum\limits_{i=t_{\text{D}}/\Delta t}^{13.8\text{ Gyr}/\Delta t} R_{\text{Ia}}(t)\Delta t} & (t_{\text{D}} \leq t \leq 13.8\text{ Gyr}) \\ 0 & (t \geq 13.8\text{ Gyr}) \end{cases} \end{aligned} \tag{27}$$

where the $\rightarrow$ denotes the switch from the analytic expression to the numerical approximation implemented in `VICE`. This implementation also takes into account a minimum delay time for SNe Ia t_{D}, prior to which there are no WD detonations. This allows users to specify any arbitrary function of time for $R_{\text{Ia}}(t)$ and they need only worry about the scaling with time in the $t_{\text{C}} \leq t \leq 13.8$ Gyr time interval.

Because stars form continuously in galaxies, the quantity of interest at any given timestep is not the enrichment rate from a given episode of star formation, but rather the sum total from all previous episodes. Under this formulation, this can be achieved by integrating over the star formation history weighted by $R_{\text{Ia}}(t)$:

$$\dot{M}_x^{\text{Ia}}(t) = y_x^{\text{Ia}} \frac{\int_0^t \dot{M}_*(t')R_{\text{Ia}}(t-t')dt'}{\int_0^\infty R_{\text{Ia}}(t')dt'} \tag{28}$$

where R_{Ia} is evaluated at $t - t'$ because this is the lookback time to the episode of star formation at time t'. We implement the following numerical approximation to this equation in `VICE`[6]:

$$\dot{M}_x^{\text{Ia}}(t) = y_x^{\text{Ia}} \sum_{i=0}^{t/\Delta t} \dot{M}_*(i\Delta t)R_{\text{Ia,reduced}}(t - i\Delta t)\Delta t \tag{29}$$

Source code can be found at https://github.com/giganano/VICE/blob/master/vice/src/sneia.c.

[6] The exact numerical implementation in `VICE` cancels the factor of Δt here with that in the denominator of $R_{\text{Ia,reduced}}$.

4.4) Asymptotic Giant Branch Stars

Asymptotic Giant Branch (AGB) stars are evolved stars that have carbon-oxygen cores surrounded by helium and hydrogen shells. These stars undergo thermal pulsations due to explosive ignition of helium fusion in the shell, generally known as helium shell flashes. During these pulses, material from the core is often mixed into the outer layers via convection, a process known as *dredge-up*. Nucleosynthesis via this channel is one of the primary sources of s-process elements in the universe.

Naively, one would expect that a delay-time distribution similar to the treatment of SNe Ia would suffice. However, this approach would implicitly adopt the assumption that every element is enriched via AGB stars with the same delay-time distribution. This is likely true for SNe Ia because white dwarves are stellar remnants; the explosion occurs generally long after the stellar envelope has been ejected. However, the AGB phase of stellar evolution occurs prior to the production of the remnant, and the yields for a given element are generally quite sensitive to the initial mass and metallicity of the star. The mass-dependence of these yields may be different from element to element, implying a different delay-time distribution for each element. We therefore adopt a different implementation in `VICE`.

Because stars of a given mass have a given lifetime (section 2.1), the lookback time to a given episode of star formation specifies the mass of the AGB stars associated with that population that are currently enriching the ISM. `VICE` operates under the approximation that the post-main sequence lifetimes of stars are instantaneous (accurate to ∼5-10%, sufficient for the single-zone approximation).

Enrichment from AGB stars is our motivation for defining the main sequence mass fraction $h(t)$ for single stellar populations. This is the fraction of a given stellar population's mass that is still in the form of main sequence stars. With $h(t)$ defined as in section 2.3, the rate of enrichment for AGB stars associated with a single stellar population is given by:

$$\dot{M}_x^{\text{AGB}} = -y_x^{\text{AGB}}(m_{\text{to}}|Z)M_*\dot{h} \tag{30}$$

where $\dot{h}$ is evaluated at the lookback time to the stellar population's formation. There is a minus sign because $h(t)$ is a monotonically decreasing function, and hence $\dot{h} < 0$. For continuous star formation, this becomes an integral over the star formation history:

$$\begin{aligned} \dot{M}_x^{\text{AGB}} &= -\int_0^t y_x^{\text{AGB}}(m_{\text{to}}(t-t')|Z(t'))\dot{M}_*(t')\dot{h}(t-t')dt' \\ &\to -\sum_{i=0}^{t/\Delta t} y_x^{\text{AGB}}(m_{\text{to}}(t-i\Delta t)|Z(i\Delta t))\dot{M}_*(i\Delta t)[h((i+1)\Delta t) - h(i\Delta t)] \end{aligned} \tag{31}$$

This equation is implemented in `VICE` with an extra factor of Δt in the summation to determine the total mass produced by AGB stars in a given timestep directly. Source code can be found at `https://github.com/giganano/VICE/blob/master/vice/src/agb.c`.

As discussed in section 2.3, the approximation $h(t) \approx 1 - r(t)$ where r is the cumulative return fraction fails at the 15% level for single stellar populations after ∼10 Gyr. This is the reason that AGB enrichment is implemented via the main sequence mass fraction rather than the cumulative return fraction.

5.1) Core Collapse Supernovae

VICE operates under an implementation of nucleosynthetic yields from core-collapse supernovae (CCSNe) that are defined as the fraction of a single stellar population's mass that is converted to some element x during massive star explosions. Letting M_x denote the mass of the element x produced by the core collapse explosion of a star with initial mass M, the yield is given by:

$$y_x^{\text{CC}} = \frac{\int_8^u M_x \frac{dN}{dm} dm}{\int_l^u M \frac{dN}{dm} dm} \tag{32}$$

VICE operates under the commonly-adopted assumption that stars more massive than 8 $M_\odot$ explode as CCSNe; hence the lower bound of the integral in the numerator. This equation is nothing more than a mathematical statement of "mass produced over total stellar mass".

Given a table of mass yields of the element x sampled on a grid of stellar masses, this equation can be evaluated by interpolating between the stellar masses on the grid. VICE includes functionality for evaluating these yields under this prescription for both Kroupa[7] and Salpeter[8] IMFs. It has the Chieffi & Limongi (2004), ApJ, 608, 405, Chieffi & Limongi (2013), ApJ, 764, 21, Limongi & Chieffi (2018), ApJS, 237, 13, and the classic Woosley & Weaver (1995), ApJS, 101, 181 tables built-in. This allows users to easily call `vice.fractional_cc_yield`, passing an element along with the desired study and a metallicity at which they report yields, and VICE will return the fractional nucleosynthetic yield determined numerically via built-in Gaussian quadrature functions. These functions are scripted in `ANSI/ISO C` and are wrapped for calling form `python`, and as such they are not dependent on any publicly available quadrature functions such as those found in `scipy`.

While VICE includes functionality for users to calculate these yields from various studies at whatever metallicities they report, the chemical evolution simulations ran by VICE know nothing about these functions. The user gets to choose the functional form of y_x^{CC} for each element, passing it directly to `vice.ccsne_yields`. They can also construct a callable `python` function accepting one parameter, which will be interpreted as the total metallicity by mass Z. In this manner, VICE allows users to calculate yields from previous studies, folding results from multiple studies together however they see fit under whatever caveats they deem necessary, and then adopt these yields directly. VICE makes no assumptions about the form of y_x^{CC} that the user would like to adopt.

In its current state, VICE evaluates this equation 32 directly given the tabulated data. This implicitly assumes that all stars above 8 $M_\odot$ explode as a CCSN, which has been shown in recent works to be a poor assumption (see the results of Sukhbold et al. (2016), ApJ, 821, 38 for details). Stellar explodability is an open question, which undermines the validity of this approach to calculating nucleosynthetic yields from CCSNe. A future update to VICE will likely include the ability for the user to specify "islands of explodability" in their yield calculations, and VICE would artificially set the mass yield of an element x to 0 in that mass range to take this into account. VICE also artificially sets the mass yield M_x to 0 at 8 $M_\odot$; this is built into all of the yield tables stored within the software. This is by design; it is an artificial addition intended to prevent numerical entries into the calculation associated with extrapolation down to 8 $M_\odot$ potentially inflating the yield unrealistically.

The core-collapse yields are stored in an instance of a subclass of the `VICE dataframe`, source code for which can be found at https://github.com/giganano/VICE/blob/master/vice/core/_data_utils.pyx. Source code for the `vice.fractional_cc_yield` function can be found at https://github.com/giganano/VICE/blob/master/vice/data/_ccsne_yields/yield_integrator.pyx. Source code for VICE's Gaussian quadrature functions can be found at https://github.com/giganano/VICE/blob/master/vice/src/quadrature.c.

[7] Kroupa (2001), MNRAS, 322, 231
[8] Salpeter (1955), ApJ, 121, 161

5.2) Type Ia Supernovae

VICE operates under an implementation of nucleosynthetic yields from type Ia supernovae (SNe Ia) that come with an associated delay-time distribution $R_{\text{Ia}}(t)$. Under this formulation, similar to the of core-collapse supernovae, VICE defines the nucleosynthetic yield from SNe Ia as the fraction of a stellar population's mass that gets converted to element x over the duty cycle of the delay-time distribution:

$$y_x^{\text{Ia}} = \frac{M_x}{M_*} \int_0^\infty R_{\text{Ia}}(t) dt \tag{33}$$

where M_x is the mass produced by a single instance of a SN Ia. While this equation is correct, it is not useful in this form. The integral over the delay-time distribution is simply the number of SNe Ia produced by the stellar population. Thus:

$$y_x^{\text{Ia}} \rightarrow M_x \frac{N_{\text{Ia}}}{M_*} \tag{34}$$

Maoz & Mannucci (2012), PASA, 29, 447 found that $N_{\text{Ia}}/M_* = (2 \pm 1) \times 10^{-3}\ M_\odot^{-1}$. That is, on average, approximately 2000 $M_\odot$ of stars must form for a given stellar population to produce a single SN Ia.

The value of M_x can be determined from the results of simulations of SNe Ia. VICE has built-in tables from the Iwamoto et al. (1999), ApJS, 125, 439 and Seitenzahl et al. (2013), MNRAS, 429, 1156 studies. Users can call `vice.single_ia_yield` to look up these values. They can also call `vice.fractional_ia_yield` to evaluate equation 34 directly.

Just like the yields from core-collapse supernovae, VICE includes functionality for users to calculate nucleosynthetic yields from previous studies, but the chemical evolution simulations that it runs known nothing about these functions. The user gets to choose whatever value of y_x^{Ia} they so choose, and pass it directly to `vice.sneia_yields`. Currently this table does not support functional attributes, meaning that unlike core-collapse nucleosynthetic yields, VICE does not allow SNe Ia yields to be functions of metallicity in its current version.

The SNe Ia yields are stored in an instance of a subclass of the `VICE dataframe`, source code for which can be found at https://github.com/giganano/VICE/blob/master/vice/core/_data_utils.pyx. Source code for the yield calculation functions can be found at https://github.com/giganano/VICE/blob/master/vice/data/_sneia_yields/yield_calculations.pyx.

5.3) Asymptotic Giant Branch Stars

Under the prescription for enrichment via asymptotic giant branch (AGB) stars as outlined in section 4.4, the yield is determined by the fraction of a star's mass that is converted to an element x. For many elements, this also varies with the initial metallicity of the star.

Because this channel of enrichment is by nature much more mathematically complex than core-collapse and type Ia supernovae, `VICE` allows very little customization in its current version. Users have the option of choosing between the Karakas (2010), MNRAS, 403, 1413 and the Cristallo et al. (2011), ApJS, 197, 17 tables. Both of these studies report yields up to $Z = 0.02$. For an adopted solar metallicity of $Z_\odot = 0.014$, this corresponds to a total metallicity [M/H] $\approx$ 0.15. Above this metallicity, we caution users that numerical artifacts may be introduced into their simulations due to linear extrapolation from yields at lower metallicities, which may not be accurate.

These tables are sampled on grid of stellar mass and metallicity, and `VICE` internally stores the fractional yields for each element from both studies. During simulations, it then determines the yield from all other masses and metallicities via linear interpolation/extrapolation between masses and metallicities on the grid.

Source code for functions which read in the yield grids from these studies can be found at `https://github.com/giganano/VICE/blob/master/vice/data/_agb_yields/grid.pyx`.

5.4) Calibration of the Total Metallicity

In simulations that track only a small number of elements, it is crucial that steps be taken to correct the total metallicity of the interstellar medium and stars, because with only a few elements, all calculations will be biased toward low abundances. This would be a purely numerical artifact. In order to correct for this, VICE adopts the following calibration of the total metallicity:

$$Z = Z_\odot \frac{\sum_i Z_i}{\sum_i Z_i^\odot} \tag{35}$$

where $Z_\odot$ is the metallicity of the sun, Z_i is the abundance of the ith element in the simulation, and $Z_i^\odot$ is the abundance of that element in the sun.

This is where the user's adopted solar metallicity enters into their simulations. We recommend $Z_\odot = 0.014$ from of the findings of Asplund et al. (2009), ARA&A, 47, 481.

`VICE history` objects automatically calibrate the metallicity for the user when they call or index the `dataframe` with "`z`" or "`[m/h]`" (case-insensitive). In the case of the metallicity by mass Z, equation 35 is evaluated. In the case of the logarithmic abundance, `VICE` solves from equation 35 in the following manner:

$$[M/H] = \log_{10}\left(\frac{Z}{Z_\odot}\right) = \log_{10}\left(\sum_i Z_i\right) - \log_{10}\left(\sum_i Z_i^\odot\right) \tag{36}$$

6) Tests

In this section we present results quantifying VICE's integration time as a function of the number of elements simulated and the timestep size. As detailed in previous sections, at each timestep, VICE determines the enrichment of all elements from all previous timesteps. As with any other time-step style integration, the amount of data to process and thus the integration time scale with the square of the number of timesteps (i.e. $T \propto (T_{\text{end}}/\Delta t)^2$).

Similarly, VICE treats every element independently. That is, the equations detailed in previous sections are not for any specific element - we purposefully did the analysis in full generality so that none of the simulation features in VICE needed to be changed to add new chemical elements. Since VICE conducts the same analysis for each element, we thus expect the integration time to scale linearly with the number of elements tracked per simulation (i.e. $T \propto N$).

Because VICE was implemented with the scientific motivation of studying the enrichment of oxygen, iron, and strontium, the first integrations were ran with these three elements, and with timesteps of Δt = 1 Myr, each simulation finished in 20.4 seconds. With these proportionalities and this calibration, we expect the following scaling relation to describe the time per integration in VICE as a function of the number of elements N, end time T_{end}, and timestep Δt:

$$T = \left(\frac{\text{Processor Speed}}{2.7\text{ GHz}}\right)^{-1} N \left(\frac{T_{\text{end}}/\Delta t}{10^4}\right)^2 (6.8\text{ seconds}) \tag{37}$$

Because 1 Myr is a relatively fine timestep, most integrations will typically not take this long. A more typical (and VICE's default) timestep size would be expected to run in 68 milliseconds per element.

In figure 2 we present numerically calculated computing times for simulations of 5, 10, 15, 20, and 25 elements between Δt = 500 kyr and 10 Myr. We overplot as dotted lines in the corresponding color the expected $N\Delta t^{-2}$ fits for each line.

We note first that for high N, this approximation underpredicts the integration time. Even though the mathematics is implemented uniformly for each element in VICE, there is still numerical overhead which increases with each element. For example, VICE will also take longer with more elements in determining the total metallicity at each timestep. Moreover, in writing output, VICE determines every [X/Y] abundance ratio - a calculation which scales with N^2. This is an effect which would be expected to mildly increase the sensitivity to the integration time for high N simulations. In practice, we find that an $N^{1.1}$ scaling performs fine for most higher N simulations.

We also note that the computed integration times deviate from the expected fit for $\Delta t \gtrsim$10 Myr. This is because at coarser timesteps, VICE becomes write-out limited rather than algorithm limited. These runs were done with output at every Δt = 10 Myr time intervals. Thus, at timesteps coarser than this, it is stopping to write output at every timestep, and in this regime, VICE transitions from algorithm-limited to write-out limited.

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7) Figures

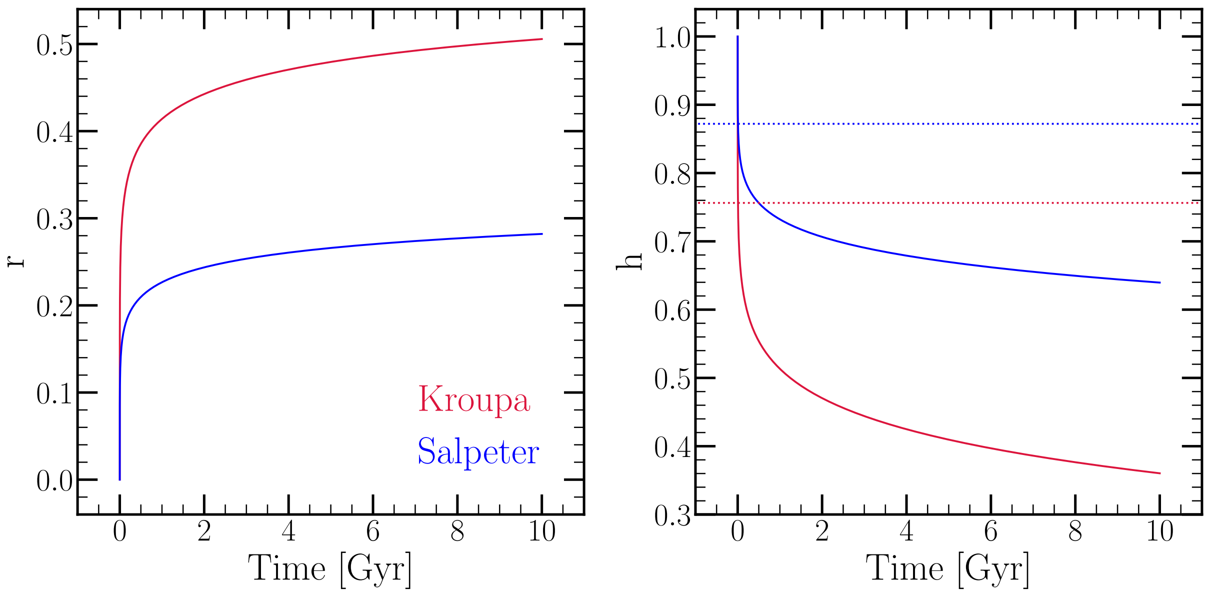

Figure 1: **Left**: The cumulative return fraction $r(t)$ as implemented in `VICE` for both Kroupa (2001), MNRAS, 322, 231 and Salpeter (1955), ApJ, 121, 161 initial mass functions (IMFs). **Right**: The main sequence mass fraction $h(t)$ as implemented in `VICE` for both Kroupa and Salpeter IMFs. The calculations presented in these figures are for lower and upper mass limits on star formation of 0.08 and 100 $M_{\odot}$. After 10 Gyr, the approximation $h(t) \approx 1 - r(t)$ fails at the ~15% level; thus `VICE` does not adopt such a formalism.

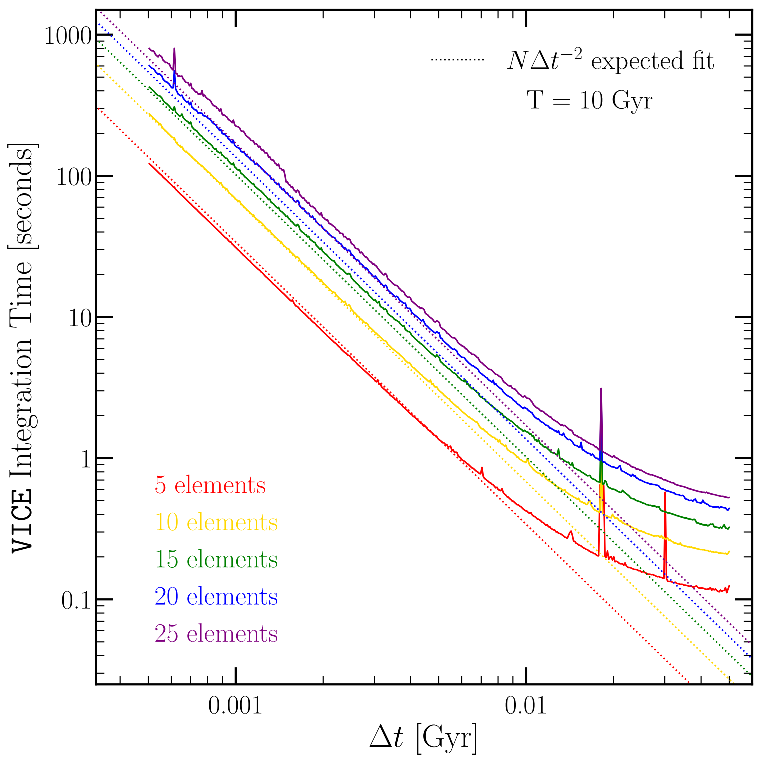

Figure 2: Timed runs with N = 5, 10, 15, 20, and 25 elements with timesteps ranging from 500 kyr to 10 Myr (solid lines) with an ending time of T = 10 Gyr. We overplot the corresponding color-coded dotted lines showing the $N\Delta t^{-2}$ expected fit. The fit does well for low N, but mildly underpredicts the integration time for higher N.