

# VICE: Versatile Integrator for Chemical Evolution

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## User's Guide

### Version 1.0.0

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VICE is open-source software released under the MIT license. We invite researchers and developers to use, modify, and redistribute however they see fit under the terms of the associated license. VICE's source code and installation instructions can be found at <http://github.com/giganano/VICE.git>. Usage of VICE leading to a publication should cite Johnson & Weinberg (2019, in prep).

*This documentation is intended to serve neither as a review of galactic chemical evolution modeling nor as a means of finding citations on previous work in this field. This provides nothing more and nothing less than standard documentation with instructions on how to use each component of the software.*

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## **1) Command Line**

I include a command-line entry with VICE, allowing users to run mathematically simple evolutionary models directly from the linux shell. While the command-line capabilities of VICE are useful for their ease, VICE is severely limited when ran in this manner in comparison to its capabilities when opened in a `python` interpreter. In this environment, users are limited to their default nucleosynthetic yield settings and smooth evolutionary models. In `python`, VICE allows users to construct arbitrary functions of time to describe many evolutionary parameters, allowing for the simulation of chemical enrichment under much more complex parameter spaces.

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## 2) The VICE dataframe

VICE provides a dataframe which can be indexed either by a column label (i.e. with a python variable of type `str`) or by row number (i.e. with a python variable of type `int`). For ease of use, indexing a VICE dataframe by column label is case-insensitive by construction.

Users can turn any python dictionary into a VICE dataframe by passing it directly to `vice.dataframe()`. There are several of these structures that I include with VICE which are designed to behave in a specific manner for various reasons specific to each case. I refer users to the documentation of each individual dataframe for further details on how they vary.

All VICE dataframes have the following functions:

### 2.1) `vice.dataframe.keys()`

Returns a list of the dataframe keys in their lower-case format. This is analogous to the `keys` function for python dictionaries.

#### Example Code

```
>>> import vice
>>> example = vice.dataframe({"oNe": 1, "Tw0": 2})
>>> example.keys()
["two", "one"]
```

**2.2) `vice.dataframe.todict()`** Returns a python dictionary analog of the dataframe. The keys to the dataframe will be entirely lower-case strings.

#### Example Code

```
>>> import vice
>>> example = vice.dataframe({"oNe": 1, "Tw0": 2})
>>> example.todict()
{"one": 1, "two": 2}
```

---

## 2.3) `vice.atomic_number`

A VICE dataframe containing the number of protons in the nucleus of each of VICE's recognized elements. By design, this dataframe does not support item assignment.

### **Example Code**

```
>>> import vice
>>> vice.atomic_number["fe"]
26
>>> vice.atomic_number["ni"]
28
>>> vice.atomic_number["au"]
79
```

---

## 2.4) `vice.ccsne_yields`

A VICE dataframe containing the current yield settings from core collapse supernovae. This dataframe is customizable and allows users to pass callable python functions, which will be interpreted as functions of metallicity  $Z$ . At the time an instance of the `singlezone` class is ran, the nucleosynthetic yield settings adopted by the simulation for each element are pulled from here.

### Example Code

```
>>> import vice
>>> vice.ccsne_yields["n"]
0.000578
>>> vice.ccsne_yields["n"] = lambda z: 0.005 * (z / 0.014)
>>> vice.ccsne_yields["n"]
<function __main__.<lambda>>>
```

### 2.4.1) `vice.ccsne_yields.factory_defaults()`

Revert the current nucleosynthetic yield settings for core collapse supernovae to their original defaults (when VICE was first installed). This will not save these settings as the new defaults; that can be achieved by calling `vice.ccsne_yields.save_defaults()` immediately following this function.

### 2.4.2) `vice.ccsne_yields.restore_defaults()`

Revert the current nucleosynthetic yield settings for core collapse supernovae to their current defaults (which may not be the original defaults). This will not save these settings as the new defaults; that can be achieved by calling `vice.ccsne_yields.save_defaults()` immediately following this function.

### 2.4.3) `vice.ccsne_yields.save_defaults()`

Save the current nucleosynthetic yield settings for core collapse supernovae as defaults. Regardless of future changes in the user's current python interpreter, calling this function will make it so that the current settings are what VICE adopts upon import.

### Notes

Saving functional yield parameters requires the python package `dill` (<https://pypi.org/project/dill/>). VICE will run properly without this package, but users will not be able to save default yields as functions of metallicity if they do not have `dill` installed.

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## 2.5) `vice.snea_yields`

### 2.5) `vice.snea_yields`

A VICE dataframe containing the current nucleosynthetic yield settings for type Ia supernovae. This dataframe is customizable but does not allow users to pass callable functions. At the time an instance of the `singlezone` class is ran, the nucleosynthetic yield settings adopted by the simulation for each element are pulled from here.

#### Example Code

```
>>> import vice
>>> vice.snea_yields["fe"]
0.00258
>>> vice.snea_yields["fe"] = 0.0017
>>> vice.snea_yields["fe"]
0.0017
>>> vice.snea_yields["fe"] = lambda z: 0.0017 * (z / 0.014)
TypeError: This dataframe does not support functional attributes.
```

#### 2.5.1) `vice.snea_yields.factory_defaults()`

Revert the current nucleosynthetic yield settings for type Ia supernovae to their original defaults (when VICE was first installed). This will not save these settings as the new defaults; that can be achieved by calling `vice.snea_yields.save_defaults()` immediately following this function.

#### 2.5.2) `vice.snea_yields.restore_defaults()`

Revert the current nucleosynthetic yield settings for type Ia supernovae to their current defaults (which may not be the original defaults). This will not save these settings as the new defaults; that can be achieved by calling `vice.snea_yields.save_defaults()` immediately following this function.

#### 2.5.3) `vice.snea_yields.save_defaults()`

Save the current nucleosynthetic yield settings from type Ia supernovae as defaults. Regardless of future changes in the user's current python interpreter, calling this functions will make it so that the current settings are what VICE adopts upon import.

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## 2.6) `vice.solar_z`

A VICE dataframe containing the abundance by mass of elements in the sun. Solar abundances are derived from Asplund et al. (2009), ARA&A, 47, 481, and have been converted into a mass fraction via:

$$Z_{x,\odot} = \mu_x X_{\odot} 10^{(X/H)-12} \quad (1)$$

where  $\mu_x$  is the mean molecular weight of the element in amu,  $X_{\odot}$  is the solar hydrogen abundance by mass, and  $(X/H) = \log_{10}(N_x/N_H) + 12$ , which is what Asplund et al. (2009) reports. For these calculations, I adopt  $X_{\odot} = 0.73$  also from Asplund et al. (2009).

This dataframe does not support user customization.

### Example Code

```
>>> import vice
>>> vice.solar_z["o"]
0.00572
>>> vice.solar_z["fe"]
0.00129
>>> vice.solar_z["fe"] = 0.0014
TypeError: This dataframe does not support item assignment.
```

---

## 2.7) `vice.sources`

A VICE dataframe containing strings denoting what astronomers generally believe to be the dominant enrichment channels for each element. These are included purely for convenience. The fields of this dataframe for each element are adopted from Johnson (2019), *Science*, 6426, 474.

### **Example Code**

```
>>> import vice
>>> vice.sources["o"]
["CCSNE"]
>>> vice.sources["fe"]
["CCSNE", "SNEIA"]
>>> vice.sources["sr"]
["CCSNE", "AGB"]
>>> vice.sources["au"]
["AGB", "NSNS"]
>>> vice.sources["au"] = ["CCSNE", "AGB"]
TypeError: This dataframe does not support item assignment.
```



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## 3.1) `vice.agb_yield_grid`

Obtain the stellar mass-metallicity grid of fractional nucleosynthetic yields from asymptotic giant branch (AGB) stars. VICE includes yields from Cristallo et al. (2011), ApJS, 197, 17 and Karakas (2010), MNRAS, 403, 1413, allowing users the choice of which to adopt in their simulations.

**Signature:** `vice.agb_yield_grid(element, study = "cristallo11")`

### Args

- `element` (Type: `str`)  
The element to obtain the yield grid for.
- `study` (Default: `"cristallo11"`; Type: `str`)  
A string [case-insensitive] denoting which AGB yield study to pull the yield table from.

### Keywords and their Associated Studies

`"cristallo11"`: Cristallo et al. (2011), ApJS, 197, 17

`"karakas10"`: Karakas (2010), MNRAS, 403, 1413

### Returns

A 3-element python list

- `returned[0]`: A 2-D python list of yields that should be indexed via `arr[mass_index][z_index]`
- `returned[1]`: A python list containing the masses in  $M_{\odot}$  that the yield grid is sampled on.
- `returned[2]`: A python list containing the metallicities by mass that the yield grid is sampled on.

### Raises

- `TypeError` if either `element` or `study` are not of type `str`.
- `ValueError` if the study or the element are not built into VICE.
- `LookupError` if `study = "karakas10"` and `vice.atomic_number[element] ≥ 29`. The Karakas (2010), MNRAS, 403, 1413 study did not report yields from AGB stars for elements heavier than nickel.
- `IOError` if both `study` and `element` are built into VICE but the data file is not found.

### Example Code

```
>>> import vice
>>> y, m, z = vice.agb_yield_grid("sr")
>>> m
[1.3, 1.5, 2.0, 2.5, 3.0, 4.0, 5.0, 6.0]
>>> z
[0.0001, 0.0003, 0.001, 0.002, 0.003, 0.006, 0.008, 0.01, 0.014, 0.02]
>>> # the fractional yield from 1.3 Msun stars at Z = 0.001
>>> y[0][2]
2.32254e-09
```

---

## 3.2) `vice.fractional_cc_yield`

Calculate an IMF-integrated fractional nucleosynthetic yield of a given element from core-collapse supernovae. VICE has built-in functions which implement Gaussian quadrature to evaluate these integrals numerically. See section 5.2 of VICE’s science documentation at <https://github.com/giganano/VICE/tree/master/docs> for further details.

**Signature:** `vice.fractional_cc_yield(element, study = “LC18”, MoverH = 0, rotation = 0, IMF = “kroupa”, method = “simpson”, lower = 0.08, upper = 100, tolerance = 1e-3, Nmin = 64, Nmax = 2e8)`

### Args

- `element` (Type: `str`)  
The element to calculate the IMF-integrated fractional yield for.
- `study` (Default: “LC18”; Type: `str`)  
A keyword [case-insensitive] denoting which study to adopt the yield from.

#### Keywords and their associated studies

- “LC18”: Limongi & Chieffi (2018), ApJS, 237, 13
- “CL13”: Chieffi & Limongi (2013), ApJ, 764, 21
- “CL04”: Chieffi & Limongi (2004), ApJ, 608, 405
- “WW95”: Woosley & Weaver (1995), ApJ, 101, 181

- `MoverH` (Default: 0; Type: real number)  
The total metallicity [M/H] of the exploding stars. There are only a handful of metallicities recognized by each study, and VICE will raise a `ValueError` if this value is not one of them.

#### Keywords and their associated metallicities

- “LC18”: [M/H] = -3, -2, -1, 0
- “CL13”: [M/H] = 0
- “CL04”: [M/H] = -inf, -4, -2, -1, -0.37, 0.15
- “WW95”: [M/H] = -inf, -4, -2, -1, 0

- `rotation` (Default: 0; Type: real number)  
The rotational velocity  $v_{\text{rot}}$  of the exploding stars in km/s. There are only a handful of rotational velocities recognized by each study, and VICE will raise a `ValueError` if this value is not one of them.

#### Keywords and their associated rotational velocities in km/s

- “LC18”:  $v_{\text{rot}}$  = 0, 150, 300
- “CL13”:  $v_{\text{rot}}$  = 0, 300
- “CL04”:  $v_{\text{rot}}$  = 0
- “WW95”:  $v_{\text{rot}}$  = 0

- `IMF` (Default: “kroupa”; Type: `str` [case-insensitive])  
The stellar initial mass function (IMF) to adopt. This must be either “kroupa” for the Kroupa (2001), MNRAS, 322, 231 study or “salpeter” for the Salpeter (1955), ApJ, 121, 161 study.

- 
- **method** (Default: “simpson”; Type: str)

The method of quadrature. See Chapter 4 of Numerical Recipes (Press, Teukolsky, Vetterling & Flannery) for details.

#### **Recognized methods**

- “simpson”
- “trapezoid”
- “midpoint”
- “euler”

- **lower** (Default: 0.08; Type: real number)

The lower mass limit on star formation in solar masses.

- **upper** (Default: 100; Type: real number)

The upper mass limit on star formation.

- **tolerance** (Default:  $10^{-3}$ ; Type: real number)

The numerical tolerance. The subroutines implementing Gaussian quadrature in VICE will not return a result until the fractional change between two successive integrations is smaller than this value.

- **Nmin** (Default: 64; Type: integer)

The minimum number of bins in quadrature.

- **Nmax** (Default:  $2 \times 10^8$ ; Type: integer)

The maximum number of bins in quadrature. Included as a failsafe against non-convergent solutions.

#### **Returns**

A 2-element python list.

- **returned[0]**: The numerically determined solution, with an estimated precision below the specified tolerance provided the solution converges within the maximum allowed number of bins in quadrature.
- **returned[1]**: The estimated fractional error.

#### **Raises**

- **TypeError** if any parameters are not of the required type.
- **ValueError** if any of the following are true:
  - The element is not built into VICE
  - The study is not built into VICE
  - The tolerance is not between 0 and 1
  - **lower** > **upper**
  - The IMF is not built into VICE
  - The method of quadrature is not built into VICE
  - **Nmin** > **Nmax**
- **LookupError** if any of the following are true:
  - The study did not report yields at the given metallicity
  - The study did not report yields at the specified rotational velocity

- 
- ScienceWarning if any of the following are true:
    - upper is larger than the largest mass on the grid reported by the specified study. VICE extrapolates to high masses in this case.
    - study is either “CL04” or “CL13” and vice.atomic\_number[element] is between 24 and 28 (inclusive). VICE warns against adopting these yields for iron peak elements.
    - Numerical quadrature did not converge within the maximum number of allowed quadrature bins

### Notes

This function evaluates the solution to the following equation under the assumption that all stars above  $8M_{\odot}$  and below the upper mass limit on star formation explode as a core collapse supernova.

$$y_x^{\text{CC}} = \frac{\int_8^u M_x \frac{dN}{dm} dm}{\int_l^u M \frac{dN}{dm} dm} \quad (2)$$

where  $M_x$  is the mass of the element  $x$  produced in the supernova of a star of initial mass  $M$ , and  $dN/dm$  is the stellar IMF.

### Example Code

```
>>> import vice
>>> y, err = vice.fractional_cc_yield("o")
>>> y
0.005643252355030168
>>> err
4.137197161389483e-06
>>> y, err = vice.fractional_cc_yield("mg", study = "CL13")
>>> y
0.000496663271667762
```

---

### 3.3) `vice.fractional_ia_yield`

Calculate an IMF-integrated fractional nucleosynthetic yield of a given element from type Ia supernovae. Unlike `vice.fractional_cc_yield`, this function does not require numerical quadrature. See section 5.2 of VICE’s science documentation at <https://github.com/giganano/VICE/tree/master/docs> for further details.

**Signature:** `vice.fractional_ia_yield(element, study = “seitenzahl13”, model = “N1”, n =  $2.2 \times 10^{-3}$ )`

#### Args

- `element` (Type: `str`)  
The symbol of the element to calculate the yield for [case-insensitive].
- `study` (Default: “seitenzahl13”; Type: `str`)  
A keyword [case-insensitive] denoting which study to adopt the yield from.

#### Keywords and their associated studies

- “seitenzahl13”: Seitzzahl et al. (2013), MNRAS, 429, 1156
- “iwamoto99”: Iwamoto et al. (1999), ApJ, 124, 439

- `model` (Default: “N1”; Type: `str`)  
The model from the associated study to adopt.

#### Keywords and their associated models

- “seitenzahl13”: N1, N3, N5, N10, N40, N100H, N100, N100L, N150, N200, N300C
- “iwamoto99”: W7, W70, WDD1, WDD2, WDD3, CDD1, CDD2

- `n` (Default:  $2.2 \times 10^{-3}$ ; Type: real number)  
The average number of type Ia supernovae produced per unit stellar mass formed  $N_{\text{Ia}}/M_*$ . This parameter has units  $M_{\odot}^{-1}$ . I recommend the default value of  $2.2 \times 10^{-3} M_{\odot}^{-1}$  in accordance with Maoz & Mannucci (2012), PASA, 29, 447.

#### Returns

The IMF-integrated yield. Unlike `vice.fractional_cc_yield`, there is no associated numerical error with this function, because the solution is analytic.

#### Raises

- `TypeError` if any parameters are not of the allowed types.
- `ValueError` if any of the following are true.
  - The element is not built into VICE
  - The study is not built into VICE
  - Parameter `n` is negative
- `LookupError` if the model is not recognized for the given study
- `IOError` if the data file is not found.

---

### **Example Code**

```
>>> import vice
>>> vice.fractional_ia_yield("fe")
0.0025825957080000002
>>> vice.fractional_ia_yield("ca")
8.935489894764334e-06
>>> vice.fractional_ia_yield("ni")
0.00016576890932800003
```

---

## 3.4) `vice.history`

Read in the part of a simulation's output that records the time-evolution of the ISM metallicity.

**Signature:** `vice.history(name)`

### Args

- `name` (Type: `str`)

The name of the output to read the history from as a string, with or without the `'vice'` extension.

### Returns

A `VICE history` object (a subclass of the `VICE dataframe`), which contains the time in Gyr, gas stellar masses in  $M_{\odot}$ , star formation and infall rates in  $M_{\odot} \text{ yr}^{-1}$ , inflow and outflow metallicities of each element, gas-phase mass and metallicities of each element, and every  $[X/Y]$  combination of abundance ratios for each output timestep.

### Raises

- `TypeError` if `name` is not of type `str`
- `IOError` if the output file is not found, is not formatted correctly, or other `VICE` output files are missing from the output. This would not happen unless the user has tampered with the output files.

### Notes

For an output under a given name, this file will be stored at `name.vice/history.out`, and it is a simple ascii text file with a comment header detailing each column. By storing the output in this manner, I allow user's to analyze the results of `VICE` simulations in languages other than `python`.

In addition to the abundance and dynamical evolution information, `history` objects will also record the effective recycling parameter and the specified mass loading parameter at all output times. These are the *actual* recycling rate divided by the star formation rate and the instantaneous mass loading  $\eta(t)$  that the user has specified regardless of the smoothing time, respectively.

In addition to the keys present in `history` `dataframes`, users may also index them with `"z"` and `"[m/h]"` [case-insensitive]. They will determine the total metallicity by mass as well as the logarithmic abundance relative to solar. Both are scaled in the following manner:

$$Z = Z_{\odot} \frac{\sum_i Z_i}{\sum_i Z_i^{\odot}} \quad (3)$$

This is the scaling of the total metallicity that is encoded into `VICE`'s timestep integrator, which prevents the simulation from behaving as if it has a systematically low metallicity when enrichment is tracked for only a small number of elements. See section 5.4 of `VICE`'s science documentation at <https://github.com/giganano/VICE/tree/master/docs> for further details.

---

### Example Code

```
>>> import vice
>>> hist = vice.history("example")
>>> hist.keys()
["z(fe)",
"mass(fe)",
"[o/fe)",
"z_in(sr)",
"z_in(fe)",
"z(sr)",
"[sr/fe)",
"z_out(o)",
"mgas",
"mass(sr)",
"z_out(sr)",
"time",
"sfr",
"z_out(fe)",
"eta_0",
"[o/sr)",
"z(o)",
"[o/h)",
"ifr",
"z_in(o)",
"ofr",
"[sr/h)",
"[fe/h)",
"r_eff",
"mass(o)",
"mstar"]
>>> print("[O/Fe] at the end of the simulation: %.2e" % (hist["[o/fe)"][-1]))
[O/Fe] at the end of the simulation: -3.12e-01
```



---

## 3.5) `vice.mdf`

Read in the normalized stellar metallicity distribution functions at the final timestep of the simulation.

**Signature:** `vice.mdf(name)`

### Args

- `name` (Type: `str`)

The name of the simulation output to read from, with or without the `‘.vice’` extension.

### Returns

A VICE `dataframe` containing bin edges and the value of the normalized stellar metallicity distribution in each  $[X/H]$  abundance and  $[X/Y]$  abundance ratio. These distributions are normalized such that the integral of the distribution over all bins is equal to 1, meaning that the recorded values should be interpreted as probability densities.

### Raises

- `TypeError` if `name` is not of type `str`
- `IOError` if the output file is not found, is not formatted correctly, or other VICE output files are missing from the output. This would not happen unless the user has tampered with the output files.

### Notes

For an output under a given name, this file will be stored at `name.vice/mdf.out`, and it is a simple ascii text file with a comment header detailing each column. By storing the output in this manner, I allow user’s to analyze the results of VICE simulations in languages other than python.

VICE normalizes stellar metallicity distribution functions such that the area under the user-specified binspace is equal to 1. Because of this, they should be interpreted as probability densities. See section 6 of VICE’s science documentation at <https://github.com/giganano/VICE/tree/master/docs> for further details.

If any  $[X/H]$  abundances or  $[X/Y]$  abundance ratios determined by VICE never pass within the user’s specified binspace, then the associated MDF will be NaN at all values.

Because the user-specified bins that the stellar MDF is sorted into may not be symmetric, if the simulation tracks the abundance ratios of stars in  $[X/Y]$ , the returned `dataframe` will *not* determine the distribution in the inverse abundance ratio  $[Y/X]$  automatically.

### Example Code

```
>>> import vice
>>> m = vice.mdf("example")
>>> m.keys()
["dn/d[sr/h],",
"dn/d[sr/fe],",
"bin_edge_left,",
"dn/d[o/h],",
"dn/d[o/fe],",
"dn/d[fe/h],",
"bin_edge_right,",
"dn/d[o/sr]"]
>>> print("dn/d[O/Fe] in 65th bin: %.2e" % (m["dn/d[o/fe]"][65]))
dn/d[O/Fe] in 65th bin: 1.41e-01
>>> print("65th bin edges: %.2e, %.2e" % (m[65]["bin_edge_left"], m[65]["bin_edge_right"]))
65th bin edges: 2.50e-01, 3.00e-01
```

---

## 3.6) vice.mirror

Obtain an instance of the `vice.singlezone` class given only an instance of the `vice.output` class. The returned `singlezone` object will have the same parameters as that which produced the output, allowing re-simulation with whatever modifications the user desires.

**Signature:** `vice.mirror(output_obj)`

### Args

- `output_obj` (Type: `vice.output`)  
Any `vice.output` object.

### Returns

A `vice.singlezone` object with the same attributes as that which produced the given output.

### Raises

- `TypeError` if `output_obj` is not an instance of the `vice.output` class.
- `ImportError` if the output has functional attributes encoded and the user does not have `dill` installed.
- `UserWarning` if the output was produced with functional attributes and the user does not have `dill` installed.

### Example Code

```
>>> import vice
>>> out = vice.output("example")
>>> new = vice.mirror(out)
>>> new.settings()
Current Settings:
=====
tau_ia -----> 1.5
recycling -----> continuous
z_solar -----> 0.014
enhancement ----> 1.0
agb_model -----> cristal1011
ria -----> plaw
delay -----> 0.15
imf -----> kroupa
smoothing -----> 0.0
schmidt_index --> 0.5
eta -----> 2.5
zin -----> 0.0
schmidt -----> False
elements -----> (u'fe', u'sr', u'o')
MgSchmidt -----> 6000000000.0
func -----> <function _DEFAULT_FUNC at 0x1109e06e0>
dt -----> 0.01
tau_star -----> 2.0
name -----> onezonemodel
m_lower -----> 0.08
m_upper -----> 100.0
Mg0 -----> 6000000000.0
```

---

```
mode -----> ifr
bins -----> [-3, -2.95, -2.9, ... , 0.9, 0.95, 1]
>>> # this reruns the simulation
>>> import numpy as np
>>> new.run(np.linspace(0, 10, 1001))
```

---

## 3.7) `vice.single_ia_yield`

Lookup the mass yield of a given element from a single instance of a type Ia supernova as determined by a given study and explosion model. See section 5.2 of VICE's science documentation at <https://github.com/giganano/VICE/tree/master/docs> for further details.

**Signature:** `vice.single_ia_yield(element, study = "seitenzahl13", model = "N1")`

### Args

- `element` (Type: `str`)  
The element to look up the yield for.
- `study` (Default: `"seitenzahl13"`; Type: `str`)  
A keyword [case-insensitive] denoting which study to adopt the yield from.

#### Keywords and their associated studies

- `"seitenzahl13"`: Seitzzahl et al. (2013), MNRAS, 429, 1156
- `"iwamoto99"`: Iwamoto et al. (1999), ApJ, 124, 439
- `model` (Default: `"N1"`; Type: `str`)  
The model from the associated study to adopt [case-insensitive].

#### Keywords and their associated models

- `"seitenzahl13"`: N1, N3, N5, N10, N40, N100H, N100, N100L, N150, N200, N300C
- `"iwamoto99"`: W7, W70, WDD1, WDD2, WDD3, CDD1, CDD2

### Returns

The mass yield of the given element in solar masses as determined for the specified model from the specified study.

### Raises

- `TypeError` if any parameters are not of the allowed types.
- `ValueError` if any of the following are true:
  - The element is not built into VICE
  - The study is not built into VICE
- `LookupError` if the model is not recognized for the given study
- `IOError` if the data file is not found

### Example Code

```
>>> import vice
>>> vice.single_ia_yield("fe")
1.17390714
>>> vice.single_ia_yield("fe", study model = "W70")
0.77516
>>> vice.single_ia_yield("ni", model = "N100L")
0.03914090000000526
```

---

## 3.8) `vice.single_stellar_population`

Simulate the nucleosynthesis of a given element from a single star cluster of given mass and metallicity. This does not take into account galactic evolution - whether or not it is depleted from inflows or ejected in winds is not considered. Only the mass of the given element produced by the star cluster is determined. See section 2.4 of VICE's science documentation for further details.

**Signature:** `vice.single_stellar_population(element, mstar = 1.e6, Z = 0.014, time = 10, dt = 0.01, m_upper = 100, m_lower = 0.08, IMF = "kroupa", RIa = "plaw", delay = 0.15, agb_model = "cristallo11")`

### Args

- **element** (Type: str)  
The symbol of the element to simulate the enrichment for [case-insensitive]
- **mstar** (Default:  $10^6$ ; Type: real number)  
The total mass of the star cluster in solar masses when it is born (at time = 0).
- **Z** (Default: 0.014; Type: real number)  
The metallicity by mass (i.e. the mass fraction of elements heavier than helium) of the stars in the cluster.
- **time** (Default: 10; Type: real number)  
The amount of time in Gyr to run the simulation for.
- **dt** (Default: 0.01; Type: real number)  
The size of each timestep in Gyr.
- **m\_upper** (Default: 100; Type: real number)  
The upper mass limit on star formation in solar masses.
- **m\_lower** (Default: 0.08; Type: real number)  
The lower mass limit on star formation in solar masses.
- **IMF** (Default: "kroupa"; Type: str)  
The stellar initial mass function (IMF) to assume as a string [case-insensitive]. Currently only "kroupa" for the Kroupa (2001), MNRAS, 322, 231 IMF and "salpeter" for the Salpeter (1955), ApJ, 121, 161 IMF are recognized.
- **RIa** (Default: "plaw"; Type: str or <function>)  
The delay-time distribution  $R_{\text{Ia}}(t)$  to adopt, where time is in Gyr. VICE will automatically normalize any function that is passed. Alternatively, VICE has built-in "plaw" (power-law,  $\propto t^{-1.1}$ ) and "exp" (exponential,  $\propto e^{-t/1.5 \text{ Gyr}}$ ) delay-time distributions.
- **delay** (Default: 0.15; Type: real number)  
The minimum delay time for the onset of type Ia supernovae in Gyr.
- **agb\_model** (Default: "cristallo11"; Type: str)  
A keyword [case-insensitive] denoting which table of nucleosynthetic yields from AGB stars to adopt.

### Recognized keywords and their associated studies

- "cristallo11": Cristallo et al. (2011), ApJS, 197, 17
- "karakas10": Karakas (2010), MNRAS, 403, 1413

---

### **Returns**

A 2-element python list.

- `returned[0]`: A python list containing the net mass of the given element produced by the star cluster at each timestep. Units are solar masses.
- `returned[1]`: A python list containing the times in Gyr corresponding to each mass yield.

### **Raises**

- `TypeError` if any parameters are not of the allowed types.
- `ValueError` if any of the following are true:
  - The element is not built into VICE
  - `mstar < 0`
  - `Z < 0`
  - `time < 0` or `time > 15`
  - `dt < 0`
  - `m_upper < 0`
  - `m_lower < 0`
  - `m_lower > m_upper`
  - The IMF is not built into VICE
  - `delay < 0`
  - `agb_model` is not built into VICE
- `LookupError` if `agb_model = "karakas10"` and `vice.atomic_number[element] ≥ 29`. The Karakas (2010), MNRAS, 403, 1413 study did not report yields for elements heavier than nickel.
- `IOError` if the AGB yield file is not found.
- `ArithmeticError` if functional RIA evaluates to a negative value, NaN, or inf at any given timestep.

### **Example Code**

```
>>> import vice
>>> mass, times = vice.single_stellar_population("sr", mstar = 1e6, Z = 0.008)
>>> # Net strontium yield of a 1e6 Msun star cluster w/metallicity Z = 0.008
>>> print("%.2e Msun" % (mass[-1]))
4.81e-02 Msun
>>> mass, times = vice.single_stellar_population("fe", mstar = 1e6)
>>> # Net iron yield of a 1e6 Msun star cluster w/metallicity Z = 0.014
>>> print("%.2e Msun" % (mass[-1]))
2.68e+03 Msun
```

---

## 4.1) `vice.singlezone`

Runs simulations of chemical enrichment under the single-zone approximation for user-specified parameters. The organizational structure of this class is simple; every attribute encodes information on a given galaxy evolution parameter. The only function in this class is the `run` function, which runs the simulation over the current settings. Sections 3, 4, and 5 of VICE’s science documentation (available at <https://github.com/giganano/VICE/tree/master/docs>) are all relevant to this class.

**Signature:** `vice.singlezone(self, name = “onezonemodel”, func = _DEFAULT_FUNC, mode = “ifr”, elements = [“fe”, “sr”, “o”], imf = “kroupa”, eta = 2.5, enhancement = 1, Zin = 0, recycling = “continuous”, bins = _DEFAULT_FUNC, delay = 0.15, dtd = “plaw”, Mg0 = 6.0e9, smoothing = 0.0, tau_ia = 1.5, tau_star = 2.0, dt = 0.01, schmidt = False, schmidt_index = 0.5, MgSchmidt = 6.0e9, m_upper = 100, m_lower = 0.08, Z_solar = 0.014, agb_model = “cristallo11”)`

### Attributes

- `name` (Default: “onezonemodel”; Type: `str`)

The name of the simulation. The output will be stored in a directory under this name with the extension “.vice”. This can also be of the form “/path/to/directory/name” and the output will be stored there. The user need not interact with any of the output files; the `vice.output` object is designed to read in all of the results automatically.

### Notes

Outputs are handled in this format because it allows users to open the files in languages other than `python`, as the simulation results are recorded in pure `ascii` text. Forcing a “.vice” extension on the name of the directory allows users to run commands in a linux kernel over all outputs in a directory via `<command> *.vice`. Within each VICE output are two “.out” files; “history.out” contains the time-evolution of the ISM metallicity and “mdf.out” contains the normed stellar metallicity distribution function. The three “.config” output files contain `python` dictionaries stored in a `pickle` with the information to reconstruct the yield settings and `singlezone` settings from the output.

- `func` (Default: `_DEFAULT_FUNC`; Type: `<function>`)

A callable `python` function of time which returns a numerical value. It must only take one parameter, which VICE will interpret as time in Gyr. The value returned by this function will represent either the gas infall history  $\dot{M}_{\text{in}}$  in  $M_{\odot} \text{ yr}^{-1}$ , the star formation history in  $\dot{M}_{*}$  in  $M_{\odot} \text{ yr}^{-1}$ , or the gas supply in  $M_{\odot}$  at that time.

### Notes

The default function returns the value 9.1 at all times. VICE defaults to infall mode, meaning that would represent an constant infall rate of  $9.1 M_{\odot} \text{ yr}^{-1}$  if neither of these parameters were changed.

See user’s notes on [functional attributes](#) and [numerical delta functions](#) in VICE.

- `mode` (Default: “ifr”; Type: `str` - either “ifr”, “sfr”, or “gas” [case-insensitive])

The interpretation of the attribute `func`. If “ifr” it represents the infall rate in  $M_{\odot} \text{ yr}^{-1}$ ; if “sfr” it represents the star formation history in  $M_{\odot} \text{ yr}^{-1}$ ; if “gas” it represents the gas supply in  $M_{\odot}$ . The argument to `func` will always be interpreted as time in Gyr.

- `elements` (Default: [“fe”, “sr”, “o”]; Type: array-like - elements of type `str` [case-insensitive])

The symbols for the elements to track the enrichment for. The more elements that are tracked, the more precisely calibrated is the total ISM metallicity at each timestep for responding to metallicity dependent nucleosynthetic yields, but the longer each simulation will take. In its current version, VICE simulates enrichment via core collapse supernovae, type Ia supernovae, and asymptotic giant branch stars for all 76 astrophysically produced elements between carbon (“c”) and bismuth (“bi”).

### Notes

VICE is compatible with the `NumPy` `array` and `Pandas` `DataFrame`, but is not dependent on either package.

- 
- **imf** (Default: “kroupa”; Type: str - either “kroupa” or “salpeter” [case-insensitive])

The assumed stellar initial mass function (IMF). VICE currently recognizes the Kroupa (2001), MNRAS, 322, 231 and Salpeter (1955), ApJ, 121, 161IMFs. A future update will likely include a wider sample of IMFs.

- **eta** (Default: 2.5; Type: real number or <function>)

The mass loading factor  $\eta = \dot{M}_{\text{out}}/\dot{M}_*$  (the ratio of the outflow to the star formation rate). This can also be a callable python function taking exactly one parameter, which will be interpreted as time in Gyr.

#### Notes

If the user changes the smoothing timescale via the attribute `smoothing`, the relationship between the outflow rate and the star formation rate becomes more complicated. See section 3.2 of VICE’s science documentation at <https://github.com/giganano/VICE/tree/master/docs> or this parameter’s docstring for mathematical and numerical details.

See user’s notes on [functional attributes](#) and [numerical delta functions](#) in VICE.

- **enhancement** (Default: 1; Type: real number or <function>)

The ratio of the outflow to ISM metallicities. This can also be a callable python function taking exactly one parameter, which will be interpreted as time in Gyr.

See user’s notes on [functional attributes](#) and [numerical delta functions](#) in VICE.

- **zin** (Default: 0; Type: real number, <function>, or python dictionary [case-insensitive])

The metallicity of gas inflow. This can either be a number, which will apply to all elements, a <function> of time in Gyr which will also apply to all elements, or a python dictionary mapping elemental symbols [VICE will respond case-insensitively] to either real numbers or callable functions of time in Gyr. This allows the user to construct arbitrary functions of time for each element, allowing them to simulate the effects of infall metallicities in full generality.

See user’s notes on [functional attributes](#) and [numerical delta functions](#) in VICE.

- **recycling** (Default: “continuous”; Type: real number or str - if str, it must be “continuous” [case-insensitive])

The cumulative return fraction  $r$ . This is the mass fraction of a single stellar population returned to the ISM as gas at the birth metallicity of the stars. By default, VICE implements continuous recycling off of a treatment of the IMF weighted by the mass of remnants as modeled by Kalirai et al. (2008), ApJ, 676, 594. If the user specifies a numerical value, it must be between 0 and 1. In this case it will represent the instantaneous recycling parameter  $r_{\text{inst}}$  as in the analytic model of Weinberg, Andrews & Freuenburg (2017), ApJ, 837, 183.

See section 3.3 of VICE’s science documentation at <https://github.com/giganano/VICE/tree/master/docs> or this parameter’s docstring for mathematical and numerical details.

- **bins** (Default: \_DEFAULT\_BINS; Type: array-like - elements are real numbers)

The bins in each [X/H] logarithmic abundance measurements and each [X/Y] abundance ratio to sort the normed stellar metallicity distribution function into. By default, VICE sorts everything into 0.05-dex width bins between [X/H] and [X/Y] = -3 and +1.

#### Notes

VICE is compatible with the NumPy array and Pandas DataFrame, but is not dependent on either package.

- **delay** (Default: 0.15; Type: real number)

The minimum delay time in Gyr for the onset of type Ia supernovae associated with each episode of star formation.



- **dtd** (Default: “plaw”; Type: str [case-insensitive] or <function>)

The delay-time distribution for type Ia supernovae to adopt. If type str, VICE will use built-in delay-time distributions (DTDs). These are “exp” for DTDs which decay exponentially with an e-folding timescale set by the attribute tau\_ia and “plaw” for a power law with index 1.1 (i.e.  $R_{\text{Ia}} \propto t^{-1.1}$ ).

Alternatively the user may pass their own function of time as  $R_{\text{Ia}}(t)$ . The user need not worry about normalizing their custom DTD; VICE will take care of that automatically.

See user’s notes on [functional attributes](#) and [numerical delta functions](#) in VICE.

- **Mg0** (Default:  $6 \times 10^9$ ; Type: real number)

The mass of the ISM gas at time  $t = 0$  in  $M_\odot$ . This parameter only matters when the simulation is in infall mode. In gas mode, func(0) specifies the initial gas supply, and in star formation mode, it is  $\text{func}(0) * \text{tau\_star}(0)$ .

- **smoothing** (Default: 0; Type: real number)

The smoothing time in Gyr to adopt. This is the timescale on which the star formation rate is time-averaged before determining the outflow rate via the mass loading parameter  $\eta$  (attribute eta).

See section 3.2 of VICE’s science documentation at <https://github.com/giganano/VICE/tree/master/docs> or this parameter’s docstring for mathematical and numerical details.

- **tau\_ia** (Default: 1.5; Type: real number)

The e-folding timescale in Gyr of an exponentially decaying delay-time distribution for type Ia supernovae. This parameter only matters when the attribute dtd = “exp”.

- **tau\_star** (Default: 2.0; Type: real number or <function>)

The star formation efficiency (SFE) timescale denoting the gas supply per unit star formation;  $\tau_* = M_g / \dot{M}_*$  in Gyr. In observational journal articles, this is sometimes referred to as the “depletion time”. This parameter is how the gas supply and star formation rate are determined off of one another at each timestep.

See user’s notes on [functional attributes](#) and [numerical delta functions](#) in VICE.

- **dt** (Default: 0.01; Type: real number)

The timestep size in Gyr. For fine timesteps with a given ending time in the simulation, this affects the total integration time with a  $\Delta t^{-2}$  dependence.

- **schmidt** (Default: False; Type: boolean)

A boolean describing whether or not to use an implementation of gas-dependent star formation efficiency (i.e. the Kennicutt-Schmidt Law; Schmidt (1959), ApJ, 129, 243; Leroy et al. (2008), AJ, 136, 2782). At each timestep, the user-specified tau\_star, normalization MgSchmidt, and schmidt\_index determine the star formation efficiency at that timestep via:

$$\tau_*^{-1} = \text{tau\_star}(t)^{-1} \left( \frac{M_g}{\text{MgSchmidt}} \right)^{\text{schmidt\_index}} \quad (4)$$

- **schmidt\_index** (Default: 0.5; Type: real number)

The power law index on star formation efficiency driven by the Kennicutt-Schmidt Law (Schmidt (1959), ApJ, 129, 243; Leroy et al. (2008), AJ, 136, 2782).

See section 3.1 of VICE’s science documentation at <https://github.com/giganano/VICE/tree/master/docs> or attribute schmidt for further details.

- 
- **MgSchmidt** (Default:  $6 \times 10^9$ ; Type: real number)

The normalization of the gas supply when the star formation efficiency is driven by the Kennicutt-Schmidt Law (Schmidt (1959), ApJ, 129, 243; Leroy et al. (2008), AJ, 136, 2782).

#### **Notes**

In practice, this quantity should be comparable to a typical gas supply of the simulated galaxy so that the actual star formation efficiency at a given timestep is near the user-specified value. See documentation for the attribute `schmidt` for further details.

- **m\_upper** (Default: 100; Type: real number)

The upper mass limit on star formation in  $M_{\odot}$ .

- **m\_lower** (Default 0.08; Type: real number)

The lower mass limit on star formation in  $M_{\odot}$ .

- **Z\_solar** (Default: 0.014; Type: real number)

The metallicity of the sun by mass. I recommend the default value of 0.014 based on the findings of Asplund et al. (2009), ARA&A, 47, 481

- **agb\_model** (Default: "crystallo11"; Type: str - either "crystallo11" or "karakas10")

A string denoting the keyword for the stellar mass-metallicity grid of yields from asymptotic giant branch (AGB) stars to adopt. In its current version, these are the only yield options for AGB stars recognized by VICE. Future updates will include a wider sample of built-in yield tables and potentially allow functions of mass and metallicity for each element.

#### **Keywords and their Associated Studies**

"crystallo11": Cristallo et al. (2011), ApJS, 197, 17

"karakas10": Karakas (2010), MNRAS, 403, 1413

#### **Functions**

[`vice.singlezon.run\(\)`](#)

---

## 4.1.1) `vice.singlezone.run()`

Runs VICE's built-in timestep integration routines over the parameters built into the attributes of this class. Whether or not the user sets `capture = True`, the output files will be produced and can be read into a `vice.output` object at any time.

**Signature:** `vice.singlezone.run(output_times, capture = False, overwrite = False)`

### Args

- `output_times` (Type: array-like - elements are real numbers)  
The times in Gyr at which VICE should record output from the simulation. These need not be sorted in any way; VICE will take care of that automatically.
- `capture` (Default = `False`; Type: `bool`)  
A boolean describing whether or not to return a `vice.output` object from the results of the simulation.
- `overwrite` (Default = `False`; Type: `bool`)  
A boolean describing whether or not to force overwrite any existing files under the same name this simulation's output files.

### Notes

In the event that `overwrite = False` (which is the default), this acts as a halting function if the user is rerunning simulations under the same name multiple times.

### Returns

If `capture = False`, this function returns nothing. If `capture = True`, this functions returns an instance of the `vice.output` class produced from this simulation's output.

### Raises

- `TypeError` if any parameters are not of the allowed types.
- `ValueError` if any element of `output_times` is negative or an inflow metallicity evaluates to a negative value at any timestep.
- `ArithmeticError` if an inflow metallicity evaluates to `NaN` or `inf` at any timestep.
- `UserWarning` if any yield settings or class attributes are callable functions and the user does not have `dill` installed.
- `ScienceWarning` if any element tracked by the simulation is enriched in significant part by the r-process, or has a weakly constrained solar abundance measurement.

### Example Code

```
>>> import vice
>>> import numpy as np
>>> example = vice.singlezone(name = "example")
>>> outtimes = np.linspace(0, 10, 1001)
>>> print(outtimes[:10])
array([0., 0.01, 0.02, 0.03, 0.04, 0.05, 0.06, 0.07, 0.08, 0.09])
>>> out = example.run(outtimes, capture = True)
>>> isinstance(out, vice.output)
True
```

---

## 4.2) `vice.output`

Reads in the output from the `vice.singlezone` class and allows the user to access it easily via VICE `dataframes`. The results are read in automatically upon instantiating an output object.

**Signature:** `vice.output(name)`

### Attributes

- `name` (Type: `str`)  
The name of the “.vice” directory containing the output of a `singlezone` object. The “.vice” extension need not be specified with the name. Upon instantiating an output object, the results will be read automatically.
- `ccsne_yields` (Type: VICE `dataframe`)  
A VICE `dataframe` containing the yield settings from core-collapse supernovae at the time the simulation was ran.
- `elements` (Type: `tuple`)  
A python `tuple` containing the symbols of the elements whose enrichment was tracked by the simulation.
- `history` (Type: VICE `dataframe`)  
A VICE `dataframe` containing the abundances at all output times as well as the time-evolution of the galaxy, such as the star formation rate, gas mass, and star formation efficiency.  
See [history](#) documentation for user’s notes on `history` objects.
- `mdf` (Type: VICE `dataframe`)  
A VICE `dataframe` containing the normalized stellar metallicity distribution function at the final timestep of the simulation. This quantity represents the probability density that a random star would have a given  $[X/H]$  abundance or  $[X/Y]$  abundance ratio in the given bin. This `dataframe` also contains the bin edges that the user built-into the `singlezone` class to run the simulation.  
See [mdf](#) documenttton for user’s notes on the recorded MDF.
- `sneia_yields` (Type: VICE `dataframe`)  
A VICE `dataframe` containing the yield settings from type Ia supernovae at the time the simulation was ran.

### Example Code

```
>>> import vice >>> out = vice.output("example")
>>> sfr = out.history["sfr"]
>>> ofe = out.history["[O/Fe]"]
>>> hundredth_line = out.history[100]
```

### Functions

[vice.output.show\(\)](#)

---

## 4.2.1) `vice.output.show()`

Show a plot of the given quantity referenced by a keyword argument [case-insensitive].

**Signature:** `vice.output.show(key)`

### Args

- `key` (Type: `str`)

The keyword argument [case-insensitive]. If this is a quantity stored in the `history` attribute, it will be plotted against time by default. Conversely, if it is stored in the `mdf` attribute, it will show the corresponding stellar metallicity distribution function.

Users can also specify an argument of the format `key1-key2` where `key1` and `key2` are elements of the `vice.output.history` dataframe. It will then plot `key1` against `key2` and show it to the user.

### Returns

This function does not return anything.

### Raises

- `TypeError` if `key` is not of type `str`
- `KeyError` if `key` is not found in either `history` or `mdf` attributes.
- `ImportError` if `matplotlib` version  $\geq 2$  is not found in the user's system.

### Notes

This function is not intended to generate publication quality plots for users. It is included purely as a convenience function for users to be able to read in and immediately inspect the results of their simulations in a plot with only a few lines of code.

This function requires `matplotlib` version  $\geq 2$ .

### Example Code

```
>>> import vice
>>> out = vice.output("example")
>>> # Will show the star formation rate against time in Gyr >>> out.show("sfr")
>>> # Will show the stellar MDF in [O/Fe]
>>> out.show("dn/d[o/fe]")
>>> # Will show the track in the [O/Fe]-[Fe/H] plane
>>> out.show("[O/Fe]-[Fe/H]")
```

---

## 5) Exception Handling

VICE provides a unique warning class: `ScienceWarning`, which inherits from `UserWarning`. This is a warning class designed to treat as a distinct set of warnings those related to the scientific accuracy or precision of values returned from any given function. Although it is not recommended, users can silence this specific class of warnings via:

```
>>> warnings.filterwarnings("ignore", category = vice.ScienceWarning)
```

Alternatively, they may silence all warnings within VICE via

```
>>> vice.warnings.filterwarnings("ignore").
```

To silence all warnings globally:

```
>>> warnings.filterwarnings("ignore")
```

Other than the `ScienceWarning`, VICE does not provide any unique exception subclasses, and operates within the python standard library framework for exception handling.

---

## 6) User's Notes

### Functional Attributes in VICE

Functional attributes in VICE must be native python functions. Any byte-compiled function, such as NumPy mathematical functions or any python code that has been ran through a Cython compiler, will produce a `TypeError`. If the user wishes to employ one of these functions, this can be achieved by simply wrapping them in a python function. For example, the following will produce a `TypeError`:

```
>>> import numpy as np
>>> import vice
>>> intgtr = vice.singlezone()
>>> intgtr.func = np.exp
```

but the following will not:

```
>>> import numpy as np
>>> import vice
>>> intgtr = vice.singlezone()
>>> def f(t):
>>>     return np.exp(t)
>>> intgtr.func = f
```

The same can be achieved with a python `lambda`.

In many instances, VICE is designed to encode functional attributes to disk memory so that they may be reloaded into python. Doing so requires the package `dill`, an extension of the python package `pickle`. If users have not already installed `dill`, it is recommended that they do so as it allows VICE to have memory of python functions that the user has saved or used in a simulation.

### Numerical Delta Functions

VICE is a timestep-style integrator, and therefore, numerical delta functions can be achieved by letting a quantity take on some very high value for one timestep. If the user wishes to build a delta function into their model, they need to make sure that:

1. They let their delta function have an intrinsic finite width of at least one timestep. Otherwise, it is not guaranteed that the numerical integrator will find the delta function.
2. They have set their output times such that VICE will write to the output file at the time of the delta function. If this is not ensured, the output will still show the behavior induced by the delta function, but potentially not in the parameter which was meant to exhibit one.

When running a simulation, I recommend that users set it to write output at every timestep for a brief period following a numerical delta function in any parameter. This simply ensures that the output will reflect more detail following its onset. See `vice.singlezone.run` documentation or docstring for details.