



Optical Strong Line Ratios Cannot Distinguish between Stellar Populations and Accreting Black Holes at High Ionization Parameters and Low Metallicities

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Abstract

High-redshift observations from JWST indicate that optical strong line ratios do not carry the same constraining power as they do at low redshifts. Critically, this prevents a differentiation between stellar and black hole accretion-driven ionization, thereby obscuring both active galactic nuclei (AGN) demographics and star formation rates. To investigate this, we compute a large suite of photoionization models with Cloudy powered by stellar populations and accreting black holes over a large grid of ages, metallicities, initial mass functions, binarities, ionization parameters, densities, and black hole masses. We use these models to test three rest-frame optical diagnostics designed to separate ionizing sources at low redshifts: the [N II]-BPT, VO87, and OHNO diagrams. We show that these diagnostics are strongly driven by the ionization parameter ($\log U$) and the gas-phase metallicity (Z_{gas}), often more so than the ionizing spectrum itself; there is significant overlap between stellar population and accreting black hole models at high $\log U$ and low Z_{gas} . The OHNO diagram is especially contaminated in the AGN region by stellar models with high $\log U$ and low Z_{gas} , consistent with high-redshift observations. We show that the [N II]-BPT, VO87, or OHNO diagrams are most sensitive to the shape of the <54 eV ionizing continuum, an energy regime in which stellar populations and black hole accretion disk models can be highly degenerate. Finally, we discuss the potential for emission lines that trace the >54 eV ionizing continuum to differentiate between ionizing sources more effectively than the [N II]-BPT, VO87, or OHNO diagrams alone.

Unified Astronomy Thesaurus concepts: Active galactic nuclei (16); Interstellar medium (847); High-redshift galaxies (734); Emission line galaxies (459); Galaxy evolution (594)

Materials only available in the online version of record: animations

1. Introduction

Reliably identifying the sources of ionizing photons is critical to properly interpreting observations of galaxies, especially at the high redshifts now accessible with JWST (J. P. Gardner et al. 2006, 2023). Misattributed emission from accreting black holes can be responsible for orders of magnitude discrepancies of derived quantities such as star formation rates and stellar masses (e.g., J. Brinchmann et al. 2004; H. Netzer et al. 2007; D. J. Rosario et al. 2013; R. L. Davies et al. 2014a, 2014b; D. J. Rosario et al. 2015; T. T. Shimizu et al. 2015; S. L. Ellison

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et al. 2016; M. Magliocchetti et al. 2016; L. M. Cairós et al. 2022; B. Wang et al. 2024, 2025a; S. Berger et al. 2025; M. Siudek et al. 2025).

There exist many different methods for constraining the presence of a luminous accreting black hole; objects for which the data support the presence of a luminous accreting black hole are referred to as “active” (or “active galactic nuclei,” AGN), and those for which the data do not have sufficient evidence are referred to as “inactive” or “star-forming.” These methods are thought to be highly dependent on viewing angle (e.g., R. Antonucci 1993; C. M. Urry & P. Padovani 1995), and range across the electromagnetic spectrum from detections of high-energy photons in the X-ray regime (e.g., Y. Q. Xue et al. 2011, 2016; B. Luo et al. 2017) to synchrotron emission in the radio (e.g., T. M. Heckman & P. N. Best 2014; P. Padovani et al. 2017). In the infrared, photometric selections have long been used to distinguish between accreting supermassive black holes and star-forming galaxies by tracing emission from hot dust largely associated with AGN (e.g., M. Lacy et al. 2004; D. Stern et al. 2005; J. L. Donley et al. 2012; A. Kirkpatrick et al. 2017, 2023).

Rest-frame optical diagnostics of ionizing sources are among the most widely used, largely due to the development of instruments designed to target rest-frame optical spectroscopy at various redshifts (e.g., D. G. York et al. 2000; I. S. McLean et al. 2012; P. Jakobsen et al. 2022). Emission lines from permitted transitions, most commonly the Balmer lines, with broad profiles ($\text{FWHM} \gtrsim 1000 \text{ km s}^{-1}$) trace the dense, rapidly moving gas which is predominantly associated with the broad-line region around a black hole, and are common diagnostic tools given the lack of other known physical conditions to produce such signatures (e.g., D. E. Osterbrock & W. G. Mathews 1986; J. W. Sulentic et al. 2000; G. Kauffmann et al. 2003; J. R. Trump et al. 2011).

For the remainder of this work, we focus on diagnostics based on the intensity ratios of strong rest-frame optical emission lines. Emission-line ratios have been used to classify ionizing sources for several decades; early studies used only a single emission-line ratio (e.g., $[\text{O III}] \lambda 5008/\text{H}\beta$) to characterize a source as a star-forming region or host of an accreting black hole (e.g., L. Searle 1971; H. E. Smith 1975; D. Alloin et al. 1978; J. M. Shuder & D. E. Osterbrock 1981). However, it was quickly shown that this one-dimensional determination was insufficient for separating Seyfert type 2 galaxies from intense starburst galaxies or shock heating (e.g., T. M. Heckman 1980; J. A. Baldwin et al. 1981; V. A. Balzano 1983; W. C. Keel 1983; D. E. Osterbrock & R. W. Pogge 1985).

The addition of a second dimension with another emission-line ratio led to “BPT” diagrams,²² which compared $[\text{O III}] \lambda 5008/\text{H}\beta$ to $[\text{N II}] \lambda 6585/\text{H}\alpha$ or $[\text{O I}] \lambda 6302/\text{H}\alpha$ (J. A. Baldwin et al. 1981). These diagnostics were designed with the criteria that (1) the line ratios be made up of strong, easily detectable lines; (2) lines that are significantly blended be avoided; (3) the wavelength separation be small, to limit effects of dust attenuation and instrumental calibrations; (4) the ratios of a forbidden line to a Balmer line be preferred, to limit abundance sensitivity; and (5) the lines used in these

diagnostics be readily accessible with current instrumentation (S. Veilleux & D. E. Osterbrock 1987).

The $[\text{N II}]$ -BPT diagnostic utilizes the ratios $[\text{O III}]/\text{H}\beta$ versus $[\text{N II}]/\text{H}\alpha$ (J. A. Baldwin et al. 1981; L. J. Kewley et al. 2001, 2006; G. Kauffmann et al. 2003; J. R. Trump et al. 2015). The original samples used to test the $[\text{N II}]$ -BPT diagnostic in J. A. Baldwin et al. (1981) included local Universe planetary nebulae, Seyfert type 1 and 2 galaxies, narrow-line radio galaxies, Herbig–Haro objects, shock-heated galaxies, and galactic and detached extragalactic H II regions. The original J. A. Baldwin et al. (1981) analysis did not make a strict demarcation for the locations of different physical sources, though it is noted that H II regions are generally lower in $[\text{O III}]/\text{H}\beta$ and $[\text{N II}]/\text{H}\alpha$ than sources ionized by other physical mechanisms (e.g., planetary nebulae and accreting black holes).

Using the photoionization modeling code MAPPINGS III (R. S. Sutherland & M. A. Dopita 1993) to model the extent of infrared starburst galaxies in emission-line ratio diagnostic space, L. J. Kewley et al. (2001) defines the extreme starburst classification on the $[\text{N II}]$ -BPT diagram as

$$\log\left(\frac{[\text{O III}]}{\text{H}\beta}\right) = \frac{0.61}{\log\left(\frac{[\text{N II}]}{\text{H}\alpha}\right) - 0.47} + 1.19, \quad (1)$$

where objects with line ratios above this curve are denoted as AGN and below this curve are denoted as star-forming.

Studies of large statistical samples of galaxies from the Sloan Digital Sky Survey (D. G. York et al. 2000) tested the $[\text{N II}]$ -BPT diagram and derived now-widely used diagnostics to separate H II regions from regions powered by accreting black holes. G. Kauffmann et al. (2003) defines the pure star formation classification,

$$\log\left(\frac{[\text{O III}]}{\text{H}\beta}\right) = \frac{0.61}{\log\left(\frac{[\text{N II}]}{\text{H}\alpha}\right) - 0.05} + 1.3, \quad (2)$$

where objects with line ratios above this curve are denoted as AGN, and below this curve are denoted as star-forming.

These two classifications are designed to probe different physical regimes of ionizing sources: the maximal extent of star formation (for the L. J. Kewley et al. 2001 diagnostic), and the region of highest purity for star formation (for the G. Kauffmann et al. 2003 diagnostic). As such, the location of a source on the $[\text{O III}]/\text{H}\beta$ versus $[\text{N II}]/\text{H}\alpha$ plane relative to these demarcations should be interpreted with their specific goals and biases in mind. Combining these two diagnostics yields a third region, that in between the two divisions, which has become known as the “composite” region (L. J. Kewley et al. 2006).

Similar to the $[\text{N II}]$ -BPT diagram, S. Veilleux & D. E. Osterbrock (1987) introduced the $[\text{O III}] \lambda 5008/\text{H}\beta$ versus $[\text{S II}] \lambda \lambda 6718, 6733/\text{H}\alpha$ diagram (dubbed “VO87”) using the criteria that (1) each line ratio be made up of strong lines; (2) lines that suffer severe blending be avoided; (3) lines should be close in wavelength, to mitigate the effects of attenuation and flux calibrations; (4) the ratios of a line of one element to a Balmer line be preferred, to limit abundance sensitivity; and (5) the lines be accessible to present instruments (at the time of S. Veilleux & D. E. Osterbrock 1987, this indicated a preference for optical over ultraviolet or other wavelength lines). The choice of $[\text{S II}]/\text{H}\alpha$ is made to alleviate potential blending of $[\text{N II}]$ and $\text{H}\alpha$ in the

²² Colloquially, the terms “BPT” or “BPT-style/BPT-like” have been used to refer to any emission-line ratio diagnostics used to separate ionizing sources. For clarity, we will refer to each of the three diagrams studied in this work explicitly: the $[\text{O III}]/\text{H}\beta$ versus $[\text{N II}]/\text{H}\alpha$ diagram as the “[N II]-BPT” diagram, the $[\text{O III}]/\text{H}\beta$ versus $[\text{S II}]/\text{H}\alpha$ diagram as the “VO87” diagram, and the $[\text{O III}]/\text{H}\beta$ versus $[\text{Ne III}]/[\text{O II}]$ diagram as the “OHNO” diagram.

traditional [N II]-BPT diagram, which can be an issue at lower spectral resolutions. S. Veilleux & D. E. Osterbrock (1987) did not give the division between H II region galaxies and AGN quantitatively for the VO87 diagram, but they do note that there are decisive regions populated by H II galaxies (low [O III]/H β and low [S II]/H α) and AGN (high [O III]/H β and high [S II]/H α).

Other works use models and large statistical samples to quantify the VO87 diagnostic, including L. J. Kewley et al. (2001, 2006) with the maximal starburst line,

$$\log\left(\frac{[\text{O III}]}{\text{H}\beta}\right) = \frac{0.72}{\log\left(\frac{[\text{S II}]}{\text{H}\alpha}\right) - 0.32} + 1.3, \quad (3)$$

and the division between AGN and low-ionization nuclear emission-line regions (LINERs),

$$\log\left(\frac{[\text{O III}]}{\text{H}\beta}\right) = \frac{0.189}{\log\left(\frac{[\text{S II}]}{\text{H}\alpha}\right)} + 0.76, \quad (4)$$

where galaxies in the low-[O III]/H β and low-[S II]/H α sector are classified as star-forming, those in the low-[O III]/H β and high-[S II]/H α sector are classified as LINERs/shocks, and those in the high-[O III]/H β region are classified as AGN.

Another diagnostic for the VO87 diagram was introduced in J. R. Trump et al. (2015), which is fashioned similarly to the G. Kauffmann et al. (2003) [N II]-BPT line, and differs from the L. J. Kewley et al. (2001, 2006) maximal starburst line in the treatment of low-metallicity H II regions, which tend to occupy the high-[O III]/H β and low-[S II]/H α sector of VO87. The J. R. Trump et al. (2015) diagnostic is defined as

$$\log\left(\frac{[\text{O III}]}{\text{H}\beta}\right) = \frac{0.48}{\log\left(\frac{[\text{S II}]}{\text{H}\alpha}\right) - 0.10} + 1.3, \quad (5)$$

where objects with line ratios above this curve are denoted as AGN, and below this curve are denoted as star-forming.

Several line ratio diagnostics have modified the criteria of the [N II]-BPT and VO87 diagrams in efforts to produce greater purity and/or completeness. Some versions leverage line ratios of nearby forbidden lines (e.g., N. J. Cleri et al. 2023a; G. Mazzolari et al. 2024; B. E. Backhaus et al. 2025), line ratios at wavelengths other than the rest-frame optical (e.g., M. G. Allen et al. 1998; A. O. Petric et al. 2011; K. Nakajima et al. 2018; M. Hirschmann et al. 2019; C. T. Richardson et al. 2022; A. Calabrò et al. 2023; A. Feltre et al. 2023; M. Hirschmann et al. 2023; S. R. Flury et al. 2025; M. Mingozzi et al. 2024, 2025), or forgo a line ratio in favor of a derived quantity, such as stellar mass (e.g., the “mass–excitation diagram”; S. Juneau et al. 2011, 2014; A. L. Coil et al. 2015), rest-frame optical and near-infrared colors (e.g., L. Trouille et al. 2011; R. Yan et al. 2011), spectral break strengths (e.g., G. Stasińska et al. 2006), equivalent widths of individual lines (e.g., R. Cid Fernandes et al. 2010), or include spatially resolved kinematics from integral field spectroscopy (IFS; e.g., P. Zhu et al. 2025).

Developed recently compared to the [N II]-BPT and VO87 diagrams, the [O III]/H β versus [Ne III] λ 3870/[O II] λ 3727, 3730 diagram (dubbed “OHNO”) was designed to separate Chandra X-ray-selected AGN from other sources at $z \sim 1$ (G. R. Zeimann et al. 2015; B. E. Backhaus et al. 2022; N. J. Cleri et al. 2023b). [Ne III]/[O II] has been used as an ionization indicator on its own (e.g., E. M. Levesque & M. L. A. Richardson 2014): The ionization

energy needed to produce [Ne III] is 40.96 eV (slightly higher than that of [O III] at 35.12 eV), and the ionization energy needed to produce [O II] is 13.62 eV, so the ratio traces ionization slightly harder than [O III]/H β .

The OHNO diagram utilizes [Ne III] and [O II], which are bluer than the H α , [N II], and [S II] complex, thus giving OHNO the potential to be used at higher redshifts. Additionally, the use of oxygen and neon lines removes the N/O abundance sensitivity of the [N II]-BPT diagram arising from the primary and secondary production pathways of nitrogen (e.g., R. B. C. Henry et al. 2000). OHNO also comes with several downsides compared to the [N II]-BPT and VO87 diagrams. First, [Ne III]/[O II] fails the criterion of the [N II]-BPT and VO87 diagrams which prefers the ratios of forbidden metal lines to Balmer lines. More critically, the fundamental physical mechanism probed by both axes of OHNO is the ionization parameter, and the similar ionization energies probed by each ratio do not offer a truly orthogonal dimension in which to separate ionizing sources (e.g., N. J. Cleri et al. 2023a, 2023b; R. L. Larson et al. 2023; B. E. Backhaus et al. 2024, 2025).

The OHNO diagnostic is defined by B. E. Backhaus et al. (2022) as

$$\log\left(\frac{[\text{O III}]}{\text{H}\beta}\right) = \frac{0.35}{2.8 \log([\text{Ne III}]/[\text{O II}]) - 0.8} + 0.64, \quad (6)$$

where it was used to show that X-ray AGN (as defined by Y. Q. Xue et al. 2011, 2016; B. Luo et al. 2017) and galaxies with very high-ionization emission lines (particularly [Ne v] λ 3427) in their spectra are preferentially classified as AGN near the peak of cosmic star formation and AGN activity at $z \sim 1$ –2 (B. E. Backhaus et al. 2022; N. J. Cleri et al. 2023b).

A common issue with most of these optical line ratio diagnostics is the lack of systematic testing through observations at high redshifts ($z > 2$). It has been shown extensively that there is evolution in the gas conditions and stellar populations in galaxies out to $z \sim 2$ (e.g., R. L. Sanders et al. 2015, 2016; A. E. Shapley et al. 2015; A. L. Strom et al. 2017; C. Papovich et al. 2022; see Section 4 for a full discussion), where the lower metallicities, higher densities, and harder ionizing radiation from star-forming galaxies may have a significant impact on the classification of ionizing sources (e.g., J. A. Baldwin et al. 1981; S. Veilleux & D. E. Osterbrock 1987; L. J. Kewley et al. 2006, 2013; S. Juneau et al. 2011, 2014; A. L. Coil et al. 2015). The lack of study beyond $z \sim 2$ is primarily due to the lack of instrumentation capable of producing high-quality rest-frame optical spectra in these early regimes prior to JWST.

With the spectroscopic capabilities and longer wavelength coverage of instruments like JWST/NIRSpec (P. Jakobsen et al. 2022), we are now able to probe the ionizing properties of early galaxies with sample sizes unmatched prior to JWST. The optical line ratio diagnostics are convenient and accessible up to $z \sim 9$, where [O III] is redshifted out of the spectral coverage of NIRSpec.

Given the ease of use for high-redshift spectra, several recent works have employed the [N II]-BPT, VO87, and OHNO diagrams at $z \gg 2$ with JWST spectroscopy. These studies have shown the potential for large amounts of contamination in both the star-forming and AGN regions of

these diagrams due to the evolving behavior of stellar populations and gas conditions across cosmic time (e.g., A. J. Cameron et al. 2023; N. J. Cleri et al. 2023a; R. L. Larson et al. 2023; R. L. Sanders et al. 2023; H. Übler et al. 2023; J. Scholtz et al. 2025; see Section 4 for a full discussion). This motivates a systematic analysis of optical line ratio diagnostics through observations in forthcoming work (N. J. Cleri et al. 2025, in preparation), and a reanalysis of the existing diagnostics of ionizing sources and their efficacy at high redshifts in this work.

In this work, we compute a library of photoionization models to test the utility of these optical strong line ratio diagnostics in preparation for large statistical samples of JWST observations at high redshifts. The remainder of this paper is structured as follows. In Section 2, we discuss the framework of our photoionization modeling. In Section 3, we analyze the [N II]-BPT, VO87, and OHNO diagrams in the context of our models. In Section 4, we discuss the implications of our results on the future use of emission-line ratio diagnostics, particularly in the context of spectroscopy of sources in the early Universe. In Section 5, we summarize the results and conclusions of this analysis.

2. Photoionization Models

For the following analysis, we use Cloudy version C23.01 (G. J. Ferland et al. 2017; C. M. Gunasekera et al. 2023). Cloudy is a photoionization simulation code designed to self-consistently model physical conditions in astrophysical clouds to predict the thermal, ionization, and chemical structure of a cloud and predict its observed spectrum. Along with this paper, we publicly release the extended Cloudy model library,²³ which includes emission-line emissivities and continua for all stellar parameters and includes additional runs for varying abundance patterns which are not included in this work.

We perform our photoionization modeling using Cloudy on the Texas A&M High Performance Research Computing (HPRC) Grace cluster,²⁴ which has 800 Intel 6248R 3.0 GHz 24-core processors with (at least) 384 Gb RAM. On a single core, the time to run a single model is of order ~ 1 minute.

We compute all of our models across a grid of ionization parameters²⁵ from $-4 < \log U < -1$ in steps of 0.25, where L. J. Kewley et al. (2019) defines the dimensionless ionization parameter U as

$$U \equiv \frac{1}{c} \frac{\Phi}{n_{\text{H}}}, \quad (7)$$

where Φ is the ionizing photon flux and n_{H} is the hydrogen density. We assume a plane-parallel gas geometry for all models, which is an unphysical but necessary simplification over a generalized geometry for a model grid of this size (H. Katz et al. 2023).

The details of the individual models used in this work are described in the following subsections.

²³ The full Cloudy model library is currently available for download at <https://njcleri.github.io/products.html> or by request to the corresponding author. The code for this work is available in Zenodo (N. Cleri 2025).

²⁴ See <https://hprc.tamu.edu/kb/User-Guides/Grace> (where the namesake of the cluster is Grace Hopper; https://en.wikipedia.org/wiki/Grace_Hopper).

²⁵ This is the initial ionization parameter Cloudy assumes at the incident face of the cloud.

Table 1
BPASS IMFs Tested in This Work

BPASS IMF	α_1	α_2	M_1 ($M_{\odot}$)	M_{max} ($M_{\odot}$)
100_300	−1.30	−2.00	0.5	300
135_300	−1.30	−2.35	0.5	300
170_300	−1.30	−2.70	0.5	300
chab300	Exp. Cutoff	−2.30	1.0	300

2.1. BPASS Stellar Population Models

The stellar population models used in this work are from the Binary Population and Spectral Synthesis (BPASS; v2.2.1) single-burst binary formation library (E. R. Stanway & J. J. Eldridge 2018). BPASS v2.2.1 has nine different initial mass functions (IMFs), which include four different high-mass slopes and high-mass cutoffs of 100 or 300 $M_{\odot}$ (where 135_300 corresponds to the BPASS default IMF; E. E. Salpeter 1955). In this work, we compute nebular-line emissivities for the IMFs listed in Table 1 (see Section 2.4 and Table 1 of E. R. Stanway & J. J. Eldridge 2018 for more details).

BPASS offers 13 different metallicities: 10^{-5} , 10^{-4} , 10^{-3} , 0.002, 0.003, 0.004, 0.005, 0.006, 0.008, 0.010, 0.014, 0.020, and 0.040, where it is taken that $0.020 = Z_{\odot}$ (recent works have suggested that $0.0225 = Z_{\odot}$, though we maintain the BPASS convention throughout this work; E. Magg et al. 2022). BPASS offers a grid of ages from $\log(\text{age}/\text{yr}) = 6.0$ to $\log(\text{age}/\text{yr}) = 11.0$ in steps of $\log(\text{age}/\text{yr}) = 0.1$. To optimize computation time, we test stellar ages in a grid of step size $\log(\text{age}/\text{yr}) = 0.1$ from $\log(\text{age}/\text{yr}) = 6.0$ to $\log(\text{age}) = 8.0$ and $\log(\text{age}/\text{yr}) = 0.5$ from $\log(\text{age}/\text{yr}) = 8.0$ to $\log(\text{age}/\text{yr}) = 11.0$, as stars of these ages in the BPASS models do have a significant ionizing photon continuum (E. R. Stanway & J. J. Eldridge 2018). We test both the single-star and binary-star populations. We use the single-burst star formation histories for all BPASS models. We assume the Cloudy default (N. Grevesse et al. 2010) solar abundance ratios and Orion dust grains for the initial gas-phase and dust abundances, with nebular metallicity scaled directly with stellar metallicity. We compute our stellar models at densities $n_{\text{H}} = 10^2, 10^3 \text{ cm}^{-3}$.

2.2. Black Hole Accretion Models

The models of black hole accretion used in this work stem from the spectral energy distributions (SEDs) of C. Done et al. (2012). These SEDs include a prescription for a blackbody accretion disk modeled as a series of blackbodies of varying temperatures as well as a Compton upscattering component from the disk, which recreates the “soft X-ray excess” often observed in local Universe sources (e.g., R. Walter & H. H. Fink 1993; C. Done et al. 2012; M. Gierliński & C. Done 2004; M. Mehdipour et al. 2015). The high-energy emission results from a second Compton upscattering in an optically thin corona above the disk, modeled by a power-law tail to the SED.

The physical parameters of the black hole accretion disk models are the XSPEC (K. A. Arnaud 1996) defaults except where specified. The black hole mass, M_{BH} , is varied over $\log M_{\text{BH}}/M_{\odot} \in \{3, 4, 5, 6, 7, 8, 9\}$. We choose to vary the black hole mass as opposed to other parameters which impact the ionizing spectrum, as the variation in black hole mass alone

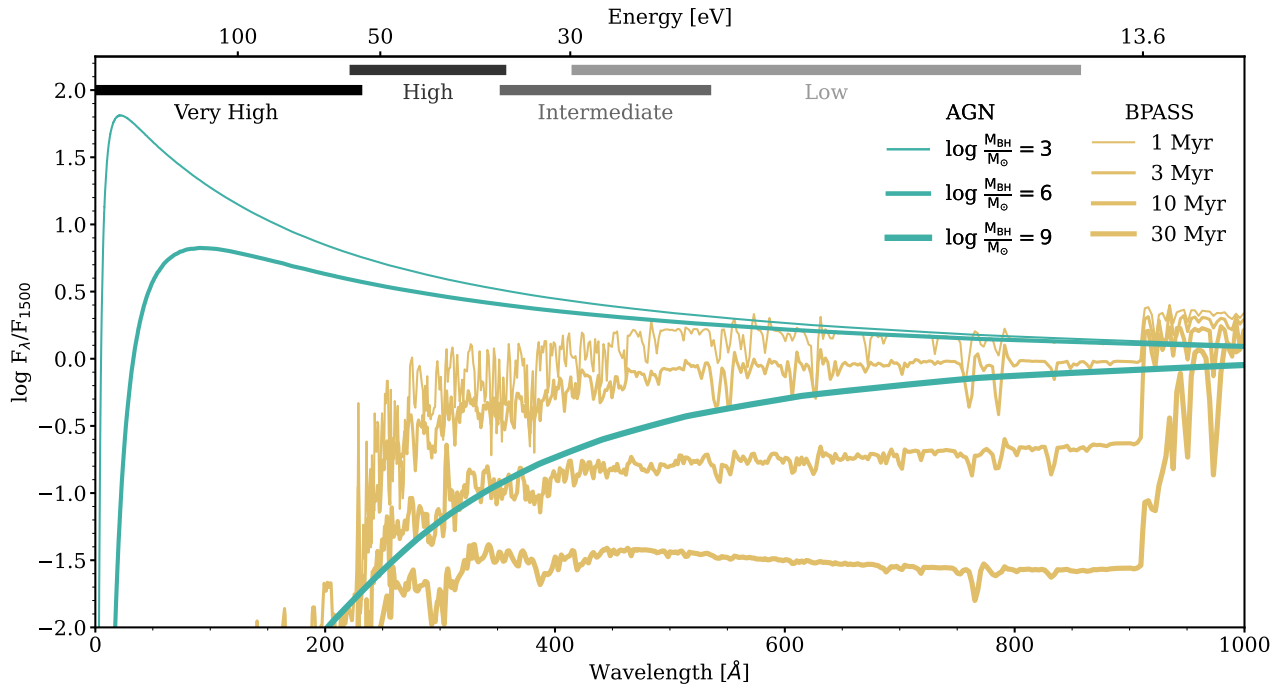


Figure 1. Example ionizing spectra of the four stellar population (gold) and three accreting black hole (blue) models used in this work. The annotations mark the four “zones” of ionization from D. A. Berg et al. (2021). The stellar populations are shown with constant IMF and metallicity with varying age, and the black hole accretion disk models are shown with constant $L_{\text{bol}}/L_{\text{Edd}}$ and spins and varying black hole masses. The full details of the models are discussed in Section 2.

spans the parameter space relevant to the line ratio diagnostics examined in this work (see Section 4.3 for discussion). The Eddington ratio is $\log L_{\text{bol}}/L_{\text{Edd}} = -1$. The corona radius is set to $10R_g$, where the gravitational radius is $R_g \equiv GM_{\text{BH}}/c^2$. The outer radius of the accretion disk is set to $\log r_{\text{out}}/R_g = 5$. The soft Comptonization component is set to $kT_e = 0.1$ keV, which is different from the XSPEC default but is chosen to maintain consistency with previous studies (J. M. Cann et al. 2018). The optical depth of the soft Comptonization component is set to $\tau = 10$. The spectral index of the hard Comptonization component is set to 10. The fraction of the power law below r_{cor} which is emitted in the hard component is set to $\log f_{\text{pl}} = -4$. The SEDs can be retrieved from XSPEC (K. A. Arnaud 1996) using the OPTXAGNF command. We compute our black hole accretion disk models at densities $n_{\text{H}} = 10^2, 10^3, 10^4 \text{ cm}^{-3}$.

The true mechanics of the emission from black hole accretion disks are highly intricate, far more so than the relatively simplistic models presented in this work (e.g., T. P. Adhikari et al. 2016; J. M. Cann et al. 2018; J. A. J. Mitchell et al. 2023; J. McKaig et al. 2023; see Section 4.3 for more discussion). Our models assume that the accretion disk ionizes a single cloud. This simplification is reasonable for this work, as models with separate broad-line region and narrow-line region physics are most likely to impact higher-energy regimes than the emission lines focused on here (i.e., $\lesssim 100$ eV; e.g., J. McKaig et al. 2023). We discuss the caveats and limitations of these models in Section 4.3.

3. Results

3.1. Analysis of Ionizing Spectra

We first examine the stellar population and black hole accretion disk ionizing spectra before being processed through Cloudy. Figure 1 shows several example ionizing spectra, including three

black hole accretion disk models of varying black hole masses ($\log M_{\text{BH}}/M_{\odot} = 3, 6, 9$) and four different BPASS stellar populations of varying ages (age = 1, 3, 10, 30 Myr). We show the four zones of ionization from D. A. Berg et al. (2021), which are defined as the ionization energies required to produce the following species:

1. Low ionization: N^+ (14.53–29.60 eV).
2. Intermediate ionization: S^{2+} (23.33–34.79 eV).
3. High ionization: O^{2+} (35.11–54.93 eV).
4. Very high ionization: He^{2+} (>54.42 eV).

Integrating the ionization spectra over the ionization zones gives the ionizing photon budget in each zone, which we denote Q_{total} (integral under the entire H-ionizing continuum), Q_{low} , $Q_{\text{intermediate}}$, Q_{high} , and Q_{veryhigh} , respectively.

Figure 2 shows the ratios of the ionizing photon budgets in each zone for the model stellar population and black hole accretion disk ionizing spectra. We choose to show only the stellar models with ages $\log \text{age}/\text{yr} \leq 8$, as the older stellar populations in BPASS do not produce appreciable amounts of ionizing photons at energies traced by the [N II]-BPT, VO87, and OHNO diagrams (E. R. Stanway & J. J. Eldridge 2018).

3.2. Inference of Model Properties from Emission-line Ratios

Figure 3 shows the three rest-optical emission-line ratios which are the focus of this work: the [N II]-BPT, VO87, and OHNO diagrams. On these diagrams we show a truncated set of our BPASS stellar populations and black hole accretion disk models, on which we perform the following analyses.

Here, we perform a simplistic Bayesian inference of the ionization parameter, gas-phase metallicity, and the ionizing photon budgets in each zone of the ionizing spectra. We

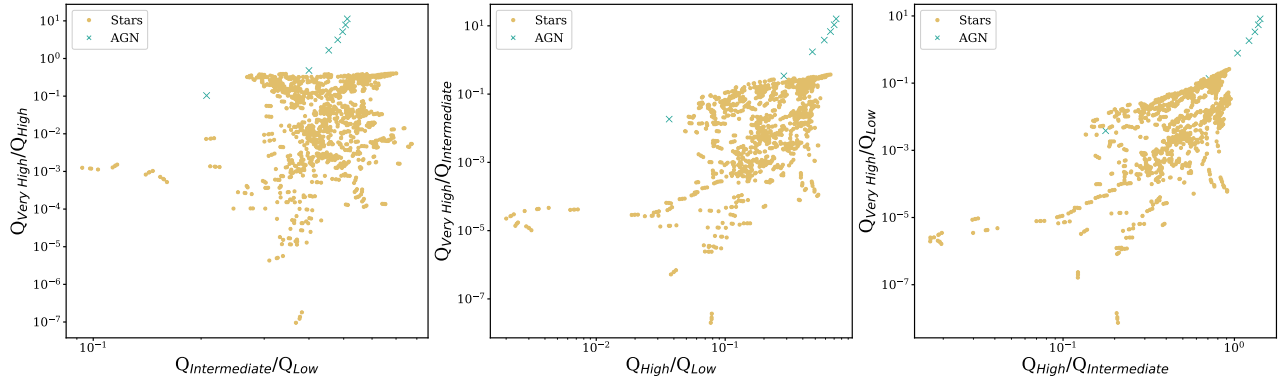


Figure 2. The ratios of ionizing photon production Q in each of the D. A. Berg et al. (2021) zones of ionization shown in Figure 1 for all of the BPASS stellar populations and black hole accretion disk ionizing spectra used in this work. We show here the stellar models of $\log \text{age}/\text{yr} < 8$, excluding the ages for which there is no significant production of photons at the energies traced by the [N II]-BPT, VO87, and OHNO diagrams.

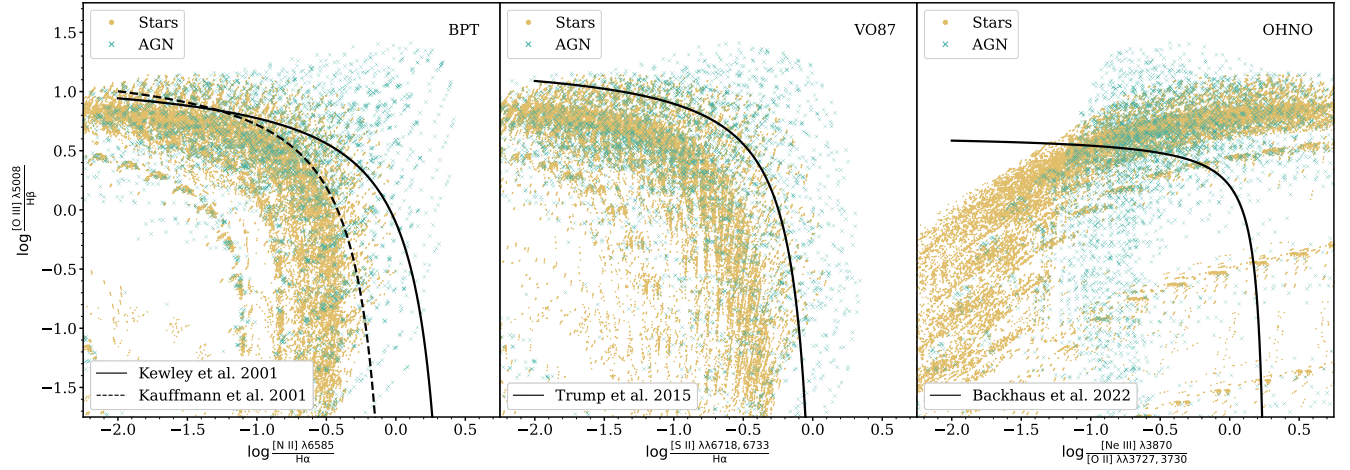


Figure 3. The [N II]-BPT (left), VO87 (center), and OHNO (right) diagrams with our suite of Cloudy models for BPASS stellar populations (gold circles) and black hole accretion disks (blue crosses). The lines show the demarcations for star formation and AGN (below and above the lines, respectively) for the [N II]-BPT (L. J. Kewley et al. 2001; G. Kauffmann et al. 2003), VO87 (J. R. Trump et al. 2015), and OHNO (B. E. Backhaus et al. 2022) diagrams, respectively. The full model parameters are described in Section 2.

calculate the log of the likelihood as a χ^2 , i.e.,

$$\log P(\text{data}|\theta) \propto -\sum_i \frac{(\text{data} - \text{model}_i)^2}{\text{uncertainty}^2}. \quad (8)$$

We perform this likelihood calculation over an evenly spaced grid (0.5 dex step size in each line ratio) in the [N II]-BPT, VO87, and OHNO planes. For eight model parameters ($\log U$, Z_{gas} , and the ratios of the ionizing photon budgets parameterized as Q_i/Q_{total} , where i indexes over the four ionization zones), we invoke uniform priors to calculate the posteriors shown in Figures 4, 5, and 6. We adopt the uncertainties to be half of the respective grid spacing (i.e., 0.25 dex in the relevant line ratio).

Figures 4, 5, and 6 show the [N II]-BPT, VO87, and OHNO diagrams, respectively, with photoionization models color-coded by ionization parameter and gas-phase metallicity. We also show the posteriors from the inference of the ionization parameter and gas-phase metallicity, with the likelihoods calculated in a discrete grid of 0.5 dex spacing in the respective line ratio plane.

Figure 7 shows the inferred properties of an observation in the [N II]-BPT plane. We choose the source GS_3073 from H. Übler et al. (2023) as a test observation, as it sits in the region of the [N II]-BPT diagram that has significant overlap

between black hole accretion disk and stellar population models at low to moderate gas-phase metallicities and high ionization parameters. GS_3073 was observed in the NIRSpec IFS GTO program “Galaxy Assembly with NIRSpec IFS,” or GA-NIFS for short (Program ID: 1216, PI: N. Lützgendorf). GS_3073 was observed with the $R \sim 1900\text{--}3600$ G395H/F290LP grating/filter pair on JWST/NIRSpec for a 5 hr integration time. GS_3073 also has well-detected broad Balmer lines, which serve as an orthogonal measure in support of the presence of an accreting massive black hole. We show the posteriors for the ionization parameter, gas-phase metallicity, and ionizing photon budget ratios. We also show the ionizing continua for the 10 most likely models, which include both young stellar populations and accreting black holes.

4. Discussion

4.1. Constraints on Nebular Conditions

Figure 3 shows the [N II]-BPT, VO87, and OHNO diagrams with a truncated set of Cloudy models discussed in Section 2. We show the extent of the stellar and accretion disk models in this parameter space, along with the impact of the dimensionless ionization parameter and the gas-phase metallicity. We show that the [N II]-BPT and VO87 diagrams do have a

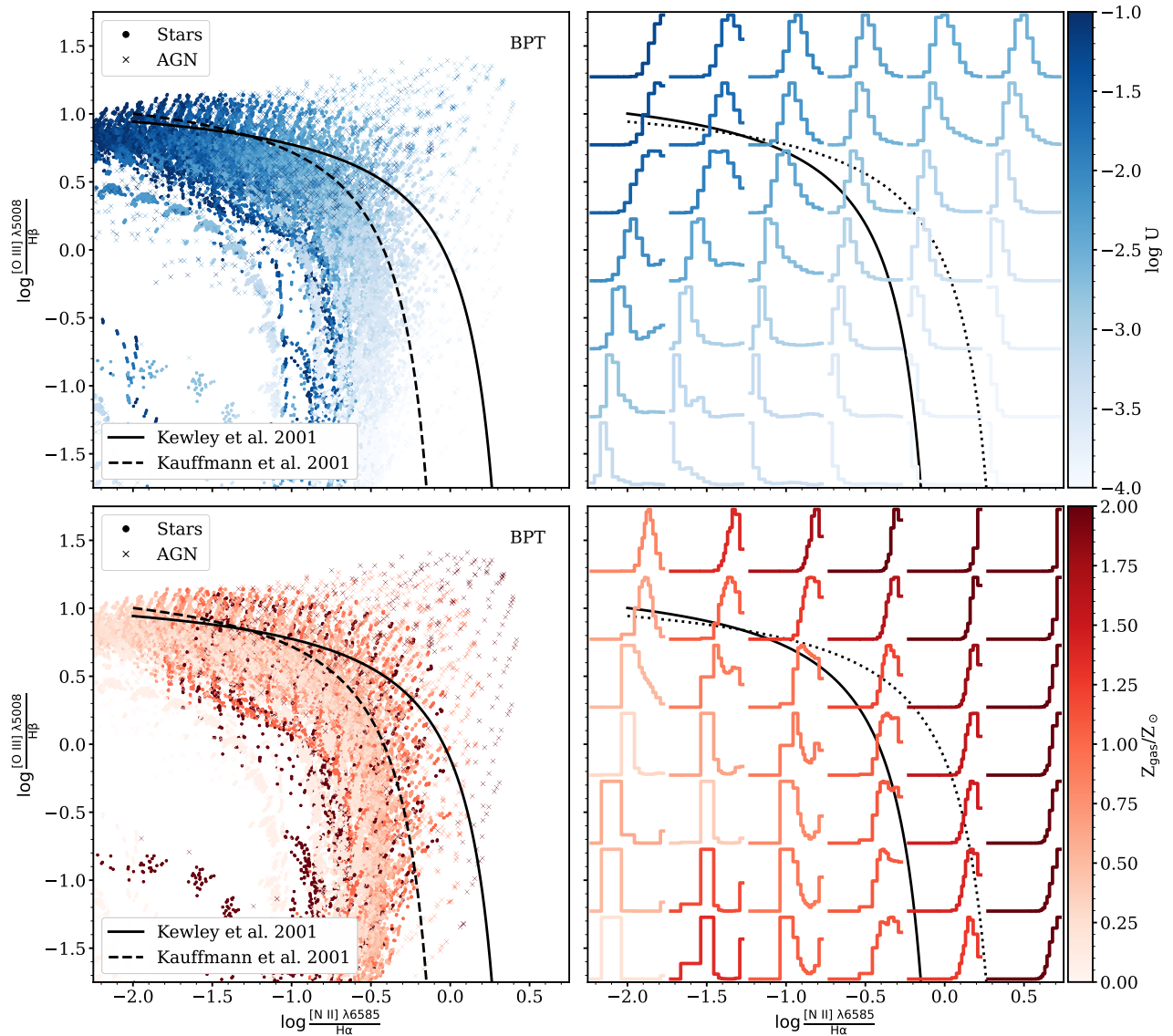


Figure 4. The [N II]-BPT diagram shown with our suite of photoionization models colored by ionization parameter (top left) and gas-phase metallicity (bottom left). The right panels show the posteriors $P(\theta|\text{data})$ for the ionization parameter (top right) and gas-phase metallicity (bottom right) for a mock observation at the respective point in the [N II]-BPT plane, where the color shows the mean of the posterior.

separation between the stellar and accretion disk models when marginalized over all model parameters, though not necessarily in line with the L. J. Kewley et al. (2001), G. Kauffmann et al. (2003), and J. R. Trump et al. (2015) diagnostics. The disagreement here is likely in the construction of the model grids in this work; we probe a very broad parameter space of stellar population models, as well as a large spread of ionization parameters and densities, designed to include the maximal extents of “normal” stellar populations potentially beyond those of the original L. J. Kewley et al. (2001, 2006) diagnostics (see Section 2). The OHNO diagram shows that the stellar models follow tracks of increasing ionization parameter across the B. E. Backhaus et al. (2022) diagnostic, with a similar extent as the black hole accretion disk models.

Figure 4 shows the inference of the nebular parameters in the [N II]-BPT diagram. This analysis reaffirms the intended physical interpretations of these ratios: The ionization parameter increases with increasing $[\text{O III}]/\text{H}\beta$, and the gas-phase metallicity increases with increasing $[\text{N II}]/\text{H}\alpha$. Figure 5 shows similar behavior in the VO87 diagram, where the

ionization parameter increases with increasing $[\text{O III}]/\text{H}\beta$ and the gas-phase metallicity increases with increasing $[\text{S II}]/\text{H}\alpha$.

Figure 6 shows the inference of the ionization parameter and nebular metallicity in the OHNO diagram. We see that the position on the OHNO diagram is most strongly driven by the ionization parameter. This is primarily due to the ionization energies needed to produce the respective emission lines: 35.12 eV and 13.62 eV for $[\text{O III}]$ and $\text{H}\beta$, and 40.96 eV and 13.62 eV for $[\text{Ne III}]$ and $[\text{O II}]$. These axes are near-completely degenerate in ionization energies probed; both $[\text{O III}]/\text{H}\beta$ and $[\text{Ne III}]/[\text{O II}]$ trace the “high” to “low” ionization ratio of the ionizing spectra, as shown in Figure 1.

We show these behaviors explicitly in Figures 8, 9, and 10 (and in the linked animations), which show the [N II]-BPT, VO87, and OHNO diagrams in a grid of ionization parameter and metallicity.

The [N II]-BPT and VO87 diagrams behave generally as predicted (e.g., J. A. Baldwin et al. 1981; S. Veilleux & D. E. Osterbrock 1987; L. J. Kewley et al. 2001, 2006, 2013, 2019; G. Kauffmann et al. 2003): A higher ionization

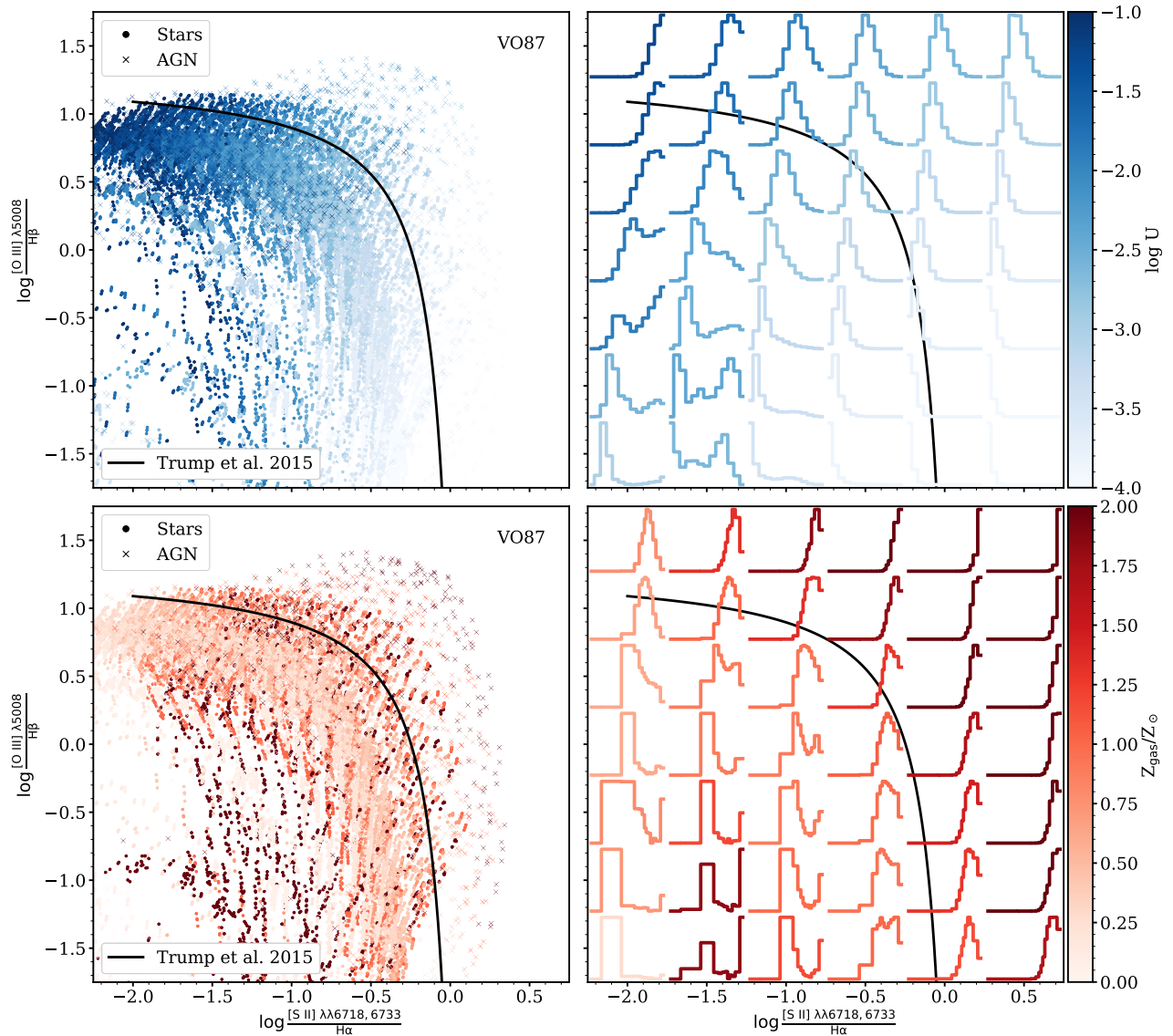


Figure 5. The VO87 diagram shown with our suite of photoionization models colored by ionization parameter (top left) and gas-phase metallicity (bottom left). The right panels show the posteriors $P(\theta|\text{data})$ for the ionization parameter (top right) and gas-phase metallicity (bottom right) for a mock observation at the respective point in the VO87 plane, where the color shows the mean of the posterior.

parameter is consistent with higher $[\text{O III}]/\text{H}\beta$ and lower $[\text{N II}]/\text{H}\alpha$ or $[\text{S II}]/\text{H}\alpha$; metallicity is less constrained, but higher metallicity is generally more consistent with higher $[\text{N II}]/\text{H}\alpha$ or $[\text{S II}]/\text{H}\alpha$. Unfortunately, Figures 8 and 9 show that there is still significant overlap and contamination of both the AGN and star-forming regions of the $[\text{N II}]\text{-BPT}$ and VO87 diagrams, particularly at lower metallicity and higher ionization parameter.

The OHNO diagram takes on a different behavior than the $[\text{N II}]\text{-BPT}$ and VO87 diagrams. The bulk of the models in the OHNO parameter space (see Figures 6 and 10) move into the AGN region at high ionization parameter ($\log U \gtrsim -2$), regardless of the stellar- or black-hole-driven ionizing spectrum. This ionization-parameter-driven contamination makes the OHNO diagram worse at separating stellar populations from accreting black holes as redshift increases. This is consistent with the interpretation of the OHNO diagram being a better diagnostic at the low redshifts for which it was first constructed ($z \sim 1$), where the star-forming regions tend to have lower ionization parameters than at the much higher redshifts probed

by JWST (e.g., B. E. Backhaus et al. 2022, 2024; N. J. Cleri et al. 2023a; D. D. Kocevski et al. 2023; R. L. Larson et al. 2023; J. R. Trump et al. 2023).

An additional complication arises from the potentially disjointed evolution and distinct nebular physics of stellar populations and accreting black holes across cosmic time, which could lead to greater scatter than what is presented in Figures 8, 9, and 10. This motivates a systematic analysis of the optical strong line ratios of high-redshift observations (N. J. Cleri et al. 2025, in preparation). We discuss the complications of redshift evolution in Section 4.4.

4.2. Constraints on the Ionizing Continuum

The critical function of line ratio diagnostics, and AGN selection as a whole, is to discern the source(s) of the ionizing continuum from the respective input data.

Figure 2 shows the ratios of the ionizing photon budgets in each of the D. A. Berg et al. (2021) ionization zones. Considering the context of the line ratios used in the $[\text{N II}]\text{-BPT}$, VO87, and

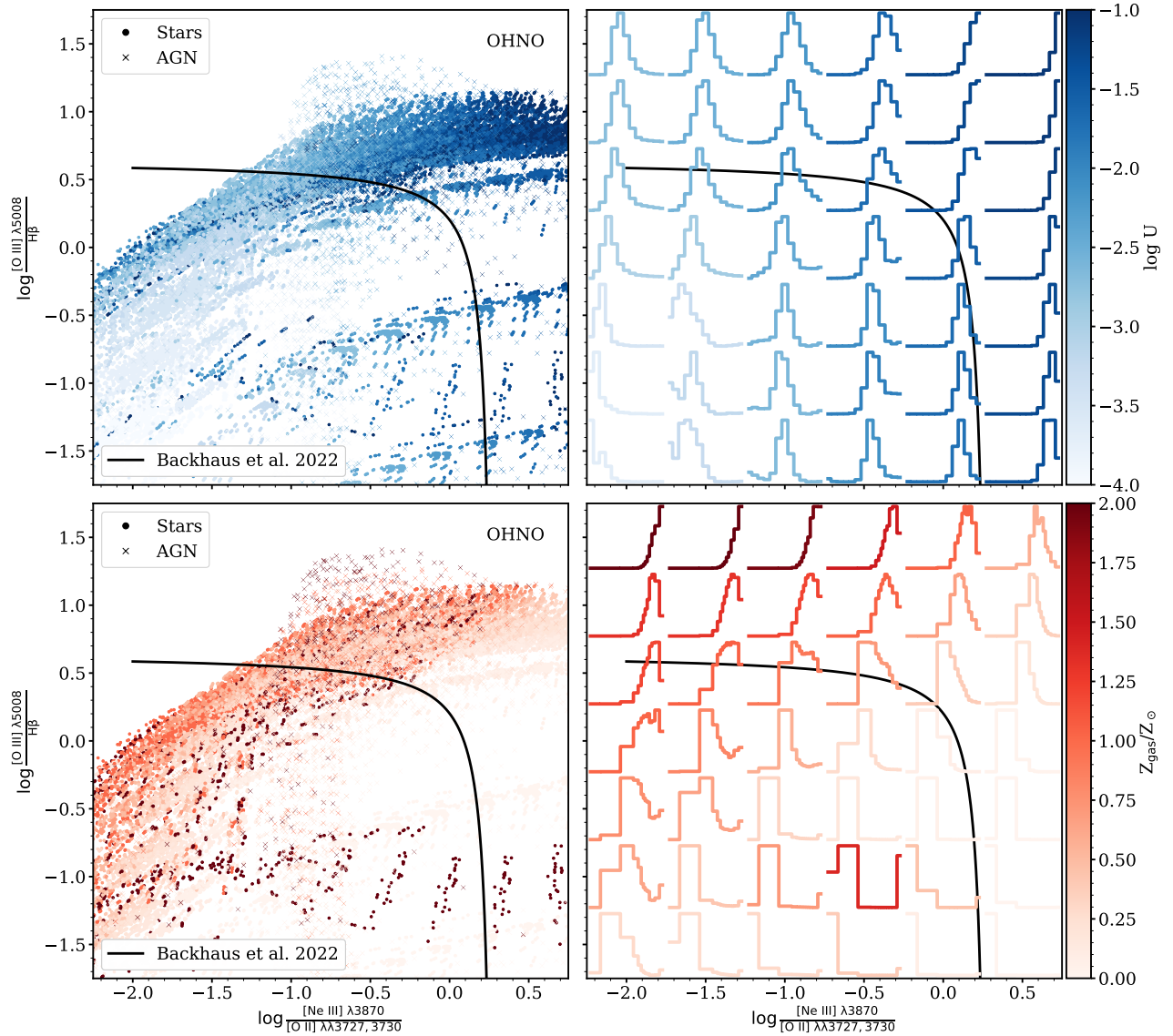


Figure 6. The OHNO diagram shown with our suite of photoionization models colored by ionization parameter (top left) and gas-phase metallicity (bottom left). The right panels show the posteriors $P(\theta|\text{data})$ for the ionization parameter (top right) and gas-phase metallicity (bottom right) for a mock observation at the respective point in the OHNO plane, where the color shows the mean of the posterior.

OHNO diagrams, the ionization zones traced by the respective line ratios are high/low ($[\text{O III}]/\text{H}\beta$, $[\text{Ne III}]/[\text{O II}]$) and low/low ($[\text{N II}]/\text{H}\alpha$, $[\text{S II}]/\text{H}\alpha$). Strictly from the ionizing continuum, there is substantial overlap between the stellar population and black hole accretion models in the $Q_{\text{high}}/Q_{\text{low}}$ regime, indicating that the shapes of the ionizing continua are similar at these energies. This is evident from the significant overlap between the stellar population and black hole accretion disk models in the $Q_{\text{high}}/Q_{\text{low}}$ regime, particularly at black hole masses in the SMBH regime ($\log M_{\text{BH}}/M_{\odot} \geq 6$), which are the most commonly observed black holes.

The models explored in this work may offer a solution not traced in the $[\text{N II}]$ -BPT, VO87, and OHNO diagrams in the form of very high-ionization emission (>54.42 eV; e.g., D. A. Berg et al. 2021). Emission lines that require >54.42 eV (e.g., He II, $[\text{Ne V}]$) trace the largest differences between stellar and black hole ionizing spectra in Figure 2, up to several orders of magnitude different in their relative ionizing photon budgets.

We show this practically using an observation of GS_3073 from H. Übler et al. (2023) in Figure 7. For GS_3073's position on the $[\text{N II}]$ -BPT diagram, we show that the most likely ionizing continua from both stellar and black hole models are similar in slope in the <54 eV regime, where the $[\text{N II}]$ -BPT, VO87, and OHNO diagrams trace. However, as shown quantitatively in Figure 2, the ionizing spectra from stellar population and black hole models are significantly different in the >54 eV regime.

Ionization-based diagnostics (e.g., $[\text{O III}]/\text{H}\beta$) are more directly tied to the shape of the ionizing continuum than ionization-insensitive nebular tracers (e.g., $[\text{N II}]/\text{H}\alpha$). By extension, adding another anchor at higher ionization (e.g., He II or $[\text{Ne V}]$) gives a more direct constraint on the shape of the ionizing spectrum than the addition of ionization-insensitive constraints. Thus, the addition of information about the production of >54 eV photons is the strongest optical constraint on the ionizing source. This is consistent with the conclusions of other works which have studied >54 eV

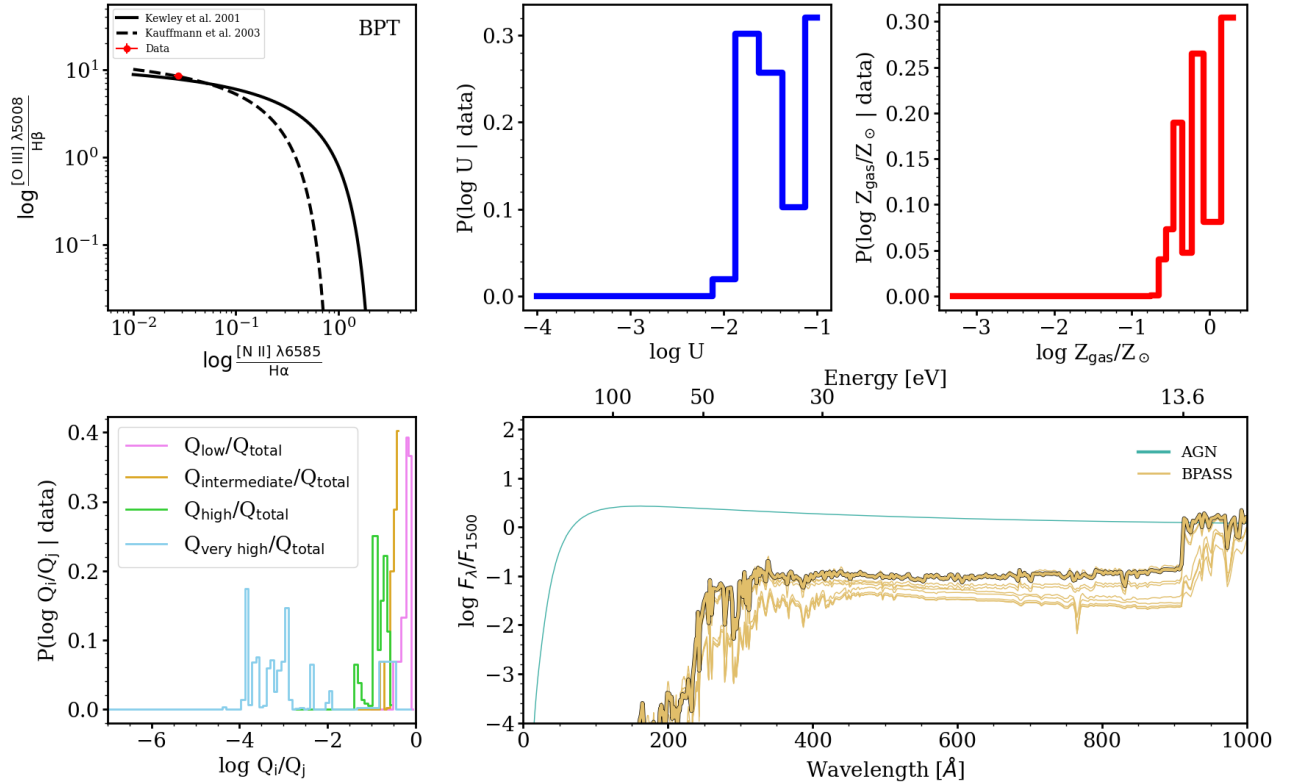


Figure 7. The inferred properties from our models for an observation in the [N II]-BPT plane, using the broad-line AGN GS_3073 from H. Übler et al. (2023) as an example. The top-left panel shows the H. Übler et al. (2023) object with 1σ uncertainties in the [N II]-BPT plane. The top-center, top-right, and bottom-left panels show the inferred ionization parameter, gas-phase metallicity, and ratios of the ionizing photon budgets in each ionization zone, respectively. The bottom-right panel shows the ionizing continua of the 10 most likely models at that point in the [N II]-BPT plane, which include both accreting black holes (blue) and stellar populations (gold). We show the ionizing continuum of the model with the highest likelihood in bold.

emission lines as a strong tracer of black hole accretion (e.g., C. De Breuck et al. 2000; N. P. Abel & S. Satyapal 2008; A. O. Petric et al. 2011; C. T. Richardson et al. 2022; N. J. Cleri et al. 2023a, 2023b; J. Chisholm et al. 2024; M. Mingozi et al. 2025; C. T. Richardson et al. 2025; P. Rinaldi et al. 2025b).

Figure 7 shows that it is difficult to uniquely constrain the source of the ionizing continuum for real observations from the [N II]-BPT diagram alone. We show that, even with the high-quality deep spectroscopy from GA-NIFS, the region of the [N II]-BPT diagram where GS_3073 falls hosts too significant of an overlap between the BPASS stellar populations and accreting black hole models to provide a unique solution for the source of the ionizing continuum. This is true even with the density of the stellar models being much higher than that of the accreting black hole models.

4.3. Caveats and Limitations

The results and conclusions of this work are subject to several caveats and limitations, which we discuss here.

An inherent issue in photoionization modeling is the sampling of parameter space. It is not expected that the full complexity of nebular physics in a galactic environment can be described in such a small number of model parameters, or that the assumptions made about aspects of the ionized medium (e.g., geometry, solar abundance scaling, etc.) are generalizable to all nebulae (see, e.g., H. Katz et al. 2023, for recent efforts toward more generalized photoionization simulations).

The stellar population model grids computed for this work were designed to cover a very broad range of stellar population properties (e.g., IMF, age, stellar metallicity, binarity) and nebular parameters (e.g., ionization parameter, gas-phase metallicity). With this choice, we probe the maximal extent of “normal” stellar populations (e.g., not Population III stars, high-mass X-ray binaries, etc.; see Section 4.3.2 for further discussion) in line ratio diagnostic space.

4.3.1. Models of Black Hole Accretion

Perhaps the most obvious limitation of this work is the simplicity and scope of the black hole accretion disk models. Black hole accretion physics is multivariate, with many physical parameters that can be changed which each affect the ionizing continuum. In this work, we vary the black hole mass, where, all else constant, increases in black hole mass lead to cooler/softer ionizing continua. Additionally, the accretion rate and black hole spin can each change the shape and normalization of the ionizing continuum. Combining these three parameters can even give extreme cases where the accretion disk gives no ionizing photons (in the case of cold lineless quasars; e.g., K. Hryniewicz et al. 2010; A. Laor & S. W. Davis 2011). We choose to limit the grid for the black hole accretion ionizing spectra to vary only the black hole mass. This choice covers the extent of the output emission-line parameters space, while saving computation time from not computing the other degenerate parameters. We also note that of the tunable parameters, black hole masses can, though with very large systematic uncertainties, be constrained by

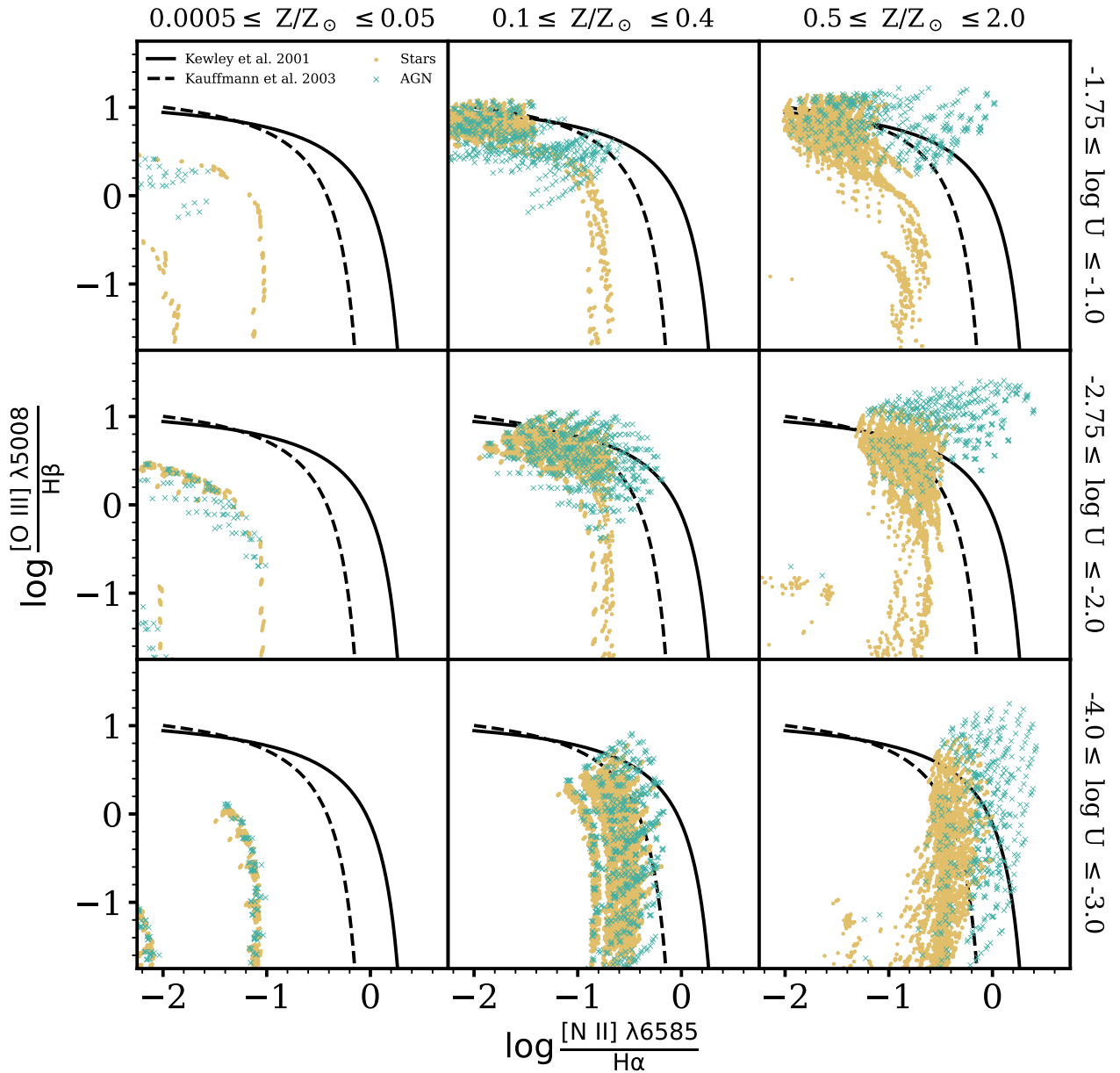


Figure 8. The [N II]-BPT diagram with our suite of Cloudy models for BPASS stellar populations (gold circles) and black hole accretion disks (blue crosses) in slices of ionization parameter (increasing up) and gas-phase metallicity (increasing to the right). The lines show the demarcations for star formation and AGN (below and above the lines, respectively) for the [N II]-BPT diagnostics from G. Kauffmann et al. (2003, dashed) and L. J. Kewley et al. (2001, solid). (Animated versions of our models on the [N II]-BPT, VO87, and OHNO diagrams are available. See Figures 11–16 in the Appendix in the online journal version or GitHub: https://github.com/njcleri/AR_05558_modeling/tree/main/figures/animations.)

spectroscopy of broad-line AGN at high redshifts (e.g., F. Pacucci et al. 2023; F. Pacucci & A. Loeb 2024; J. Matthee et al. 2025; A. J. Taylor et al. 2025a, 2025b).

Many often-used accretion disk SED models are some permutation of a broken power law, such as that from W. G. Mathews & G. J. Ferland (1987),²⁶ similar to a typical radio-quiet AGN. In the optical, this continuum corresponds to a simple power law with slope $\alpha = -1$.

Other often-used models include those of well-studied local active galaxies, including the nearby Seyfert type 1 galaxy NGC 5548 (M. Mehdipour et al. 2015). NGC 5548 has a

multiwavelength SED from near-infrared to the hard (200 keV) X-ray. The ultraviolet to near-infrared continuum of NGC 5548 is consistent with a single Comptonized disk component, with no evidence of an additional purely thermal disk component or additional component of reprocessing from the disk. NGC 5548 also exhibits a “soft X-ray excess” often seen in local AGN (e.g., C. Done et al. 2012; M. Mehdipour et al. 2015). NGC 5548 has a central engine powered by a $6.5 \times 10^7 M_\odot$ supermassive black hole (M. C. Bentz et al. 2007), and the SED has a shape consistent with a black hole of this mass in the models described in Section 2 of this work (see also N. J. Cleri et al. 2023a).

Several works suggest other empirical SED shapes for low-redshift Seyferts (L. Binette et al. 1989; J. Clavel et al. 1990) or high-redshift quasars (K. Korista et al. 1997; W. Zheng et al. 1997;

²⁶ The AGN SED default in Cloudy (accessed via the `table agn` command) differs from the W. G. Mathews & G. J. Ferland (1987) template only in the $10 \mu\text{m}$ break, which does not affect the analyses of this work (see version C17.01 of the G. J. Ferland et al. 2017 documentation for more information).

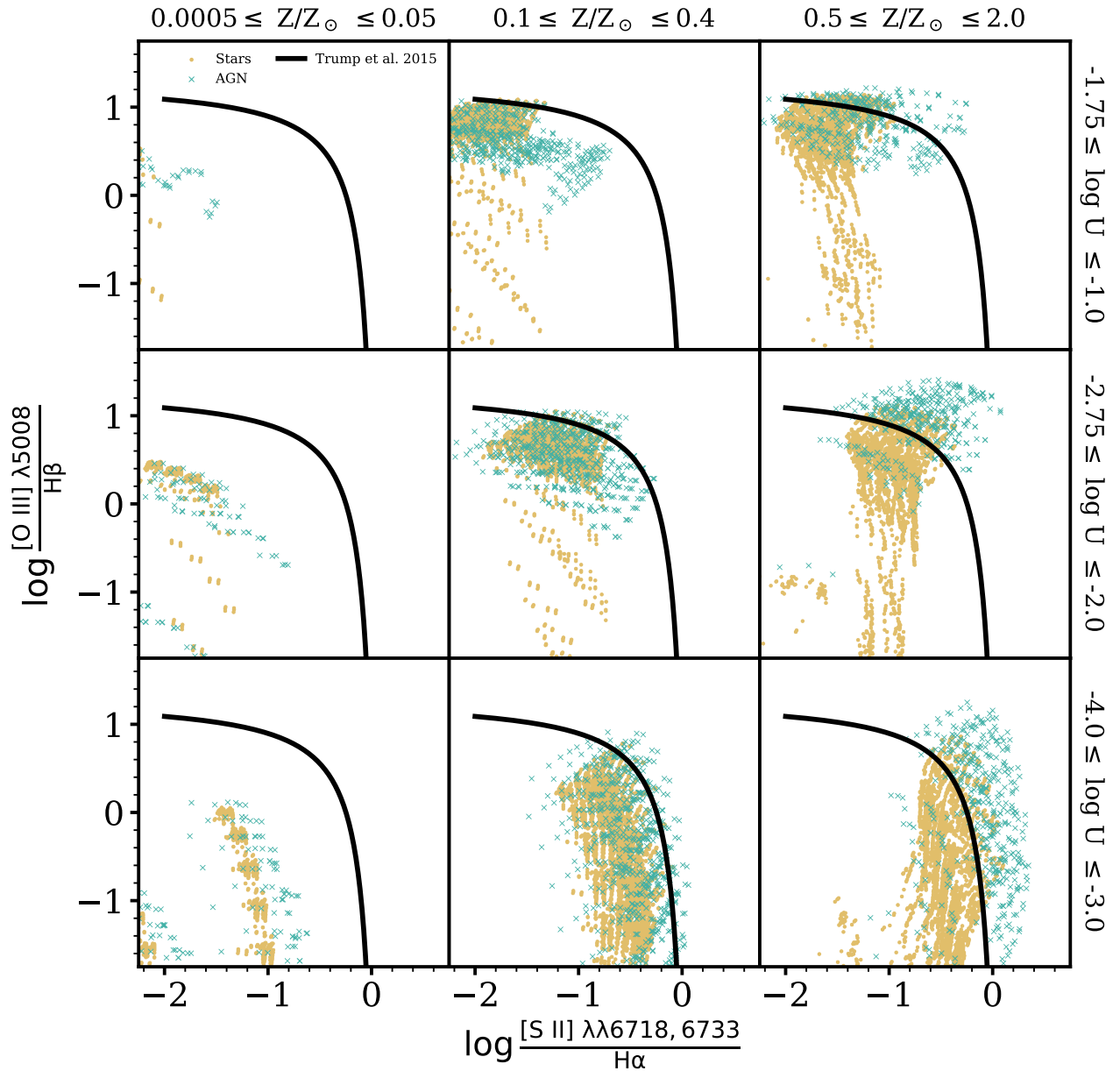


Figure 9. The VO87 diagram with our suite of Cloudy models for BPASS stellar populations (gold circles) and black hole accretion disks (blue crosses) in slices of ionization parameter (increasing up) and gas-phase metallicity (increasing to the right). The lines show the demarcations for star formation and AGN (below and above the lines, respectively) for the VO87 diagnostic from J. R. Trump et al. (2015).

D. E. Vanden Berk et al. 2001; X. Fan et al. 2006; G. T. Richards et al. 2006), yet these models are all broadly similar in shape to the C. Done et al. (2012) SEDs. There also exist many AGN which are not well described by the C. Done et al. (2012) SEDs or similar models, including low-luminosity AGN (e.g., L. C. Ho 2008), and the recently discovered “little red dots” at higher redshifts from JWST spectra (e.g., J. Matthee et al. 2024; B. Wang et al. 2024; D. D. Kocevski et al. 2023; E. Durodola et al. 2025; R. E. Hviding et al. 2025; D. D. Kocevski et al. 2025; A. J. Taylor et al. 2025a, 2025b; B. Wang et al. 2025a, 2025b).

4.3.2. Other Sources of Ionizing Photons

The model grid used in this work is limited to BPASS stellar populations and black hole accretion disk models. There exist many other potential sources of ionizing radiation which only

serve to add to the confusion in these optical strong line ratio diagnostics.

Shocks represent the most confounding source of emission-line production not explored in this work (e.g., C. F. McKee & D. J. Hollenbach 1980; G. J. Ferland & H. Netzer 1983; B. T. Draine & C. F. McKee 1993; M. A. Dopita & R. S. Sutherland 1995). Shocks have many origins, including mergers (e.g., A. M. Medling et al. 2015) and stellar winds associated with Wolf-Rayet stars (e.g., J. P. Simpson et al. 2007). Stellar winds driven by starbursts are often observed in higher-redshift galaxies with higher star formation rates than galaxies in the low-redshift Universe (e.g., B. J. Weiner et al. 2009; C. C. Steidel et al. 2010; Y. I. Izotov et al. 2012, 2021; J. Chisholm et al. 2018; J. R. Rigby et al. 2018; R. L. Davies et al. 2019, 2024). Shocks with velocities of several hundred kilometers per second can be produced by a combination of starburst-driven winds and supernovae or from outflows

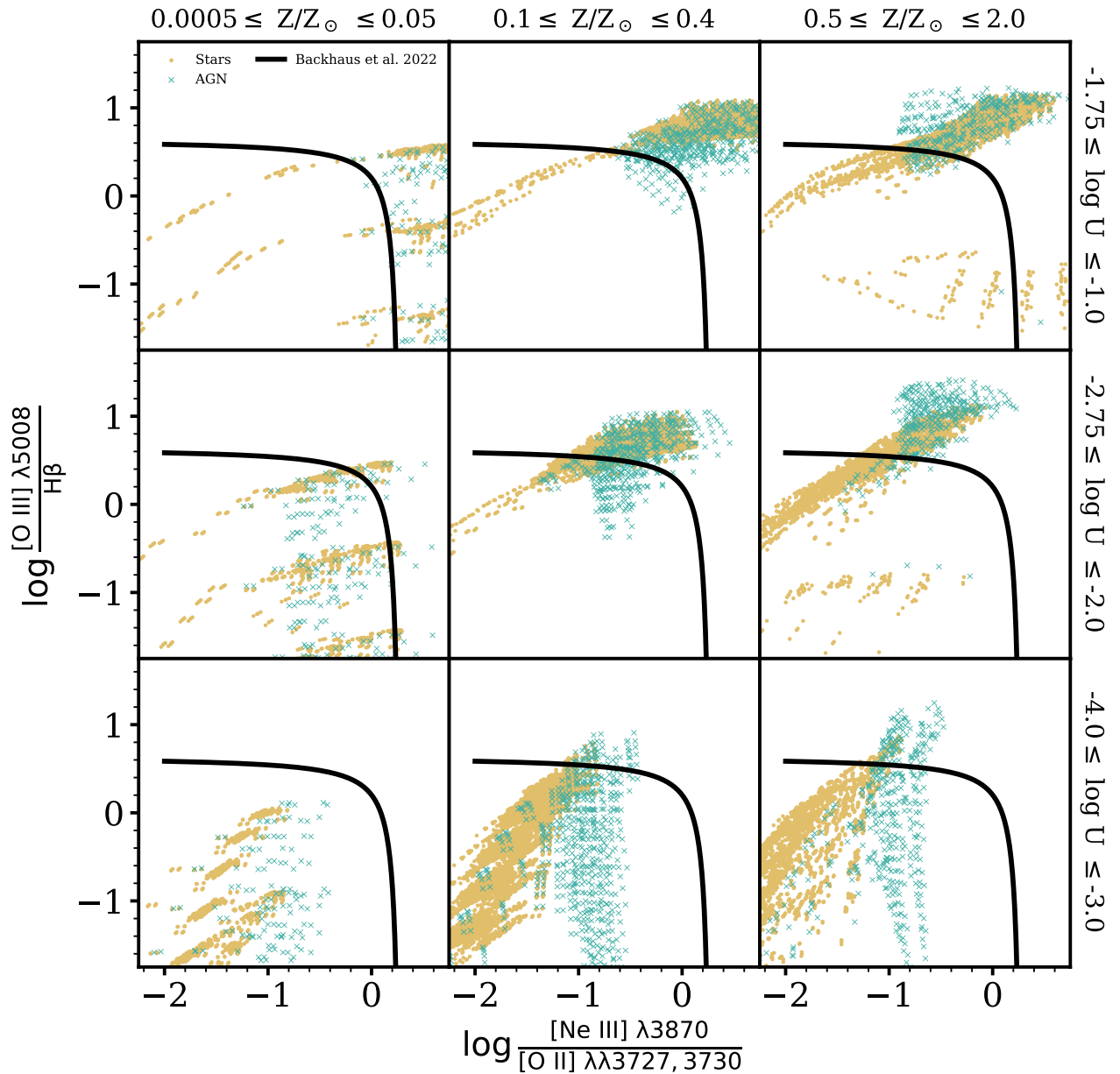


Figure 10. The OHNO diagram with our suite of Cloudy models for BPASS stellar populations (gold circles) and black hole accretion disks (blue crosses) in slices of ionization parameter (increasing up) and gas-phase metallicity (increasing to the right). The lines show the demarcations for star formation and AGN (below and above the lines, respectively) for the OHNO diagnostic from B. E. Backhaus et al. (2022).

originating from an accreting black hole (e.g., I. Evans et al. 1999; S. Veilleux et al. 2005, 2023; A. Vayner et al. 2023). Shocks have been modeled extensively (e.g., M. A. Dopita & R. S. Sutherland 1995; T. X. Thuan & Y. I. Izotov 2005; Y. I. Izotov et al. 2012, 2021), and have been shown to cover a large parameter space of optical line ratio diagnostics (e.g., the [N II]-BPT and VO87 diagrams; M. A. Dopita & R. S. Sutherland 1995).

Accreting stellar-mass compact objects, e.g., X-ray binaries, are another potential source of high-energy ionizing photons (e.g., K. Garofali et al. 2024). The impact of high-mass X-ray binaries (HMXBs) on the ionizing photon budget of a galaxy and the observed spectrum has been disputed (e.g., P. Senchyna et al. 2017; D. Schaerer et al. 2019), though HMXBs may play an important role in the production of higher-energy emission features, particularly He II (e.g., M. Shirazi &

J. Brinchmann 2012; A. E. Jaskot & M. S. Oey 2013; C. T. Richardson et al. 2025).

4.3.3. Composite Ionization

The results presented in this work represent the simplest case, where ionizing radiation comes only from a single source ionizing a single cloud, i.e., all from star formation or all from black hole accretion. A more physical interpretation is that all galaxies are, to varying degrees, composite in the sources of their ionizing radiation, meaning that there may be multiple processes ongoing simultaneously contributing to the ionizing photon budget. A first-order approximation of composite emission can be made by taking linear combinations of the emission from the single-source single-cloud models presented here, which will be studied in forthcoming work (N. J. Cleri et al. 2025, in preparation).

Other works have parameterized the composite nature of ionizing sources through the fractional contribution of black hole accretion into the ionizing photon budget (often denoted f_{AGN}). C. T. Richardson et al. (2025) present photoionization models used to test rest-frame ultraviolet, optical, and infrared diagnostic line ratios for their sensitivity to black hole mass and f_{AGN} . They find that as the ionization parameter and f_{AGN} increase in their models, the black hole mass shows a stronger influence on the predicted emission lines. They note that key lines in the rest-frame optical include He II $\lambda 4687$, which traces the thermal emission from the accretion disk at >54 eV, along with [O I] $\lambda 6302$ and the [S II] $\lambda \lambda 6718, 6733$ doublet, which are sensitive to the soft X-ray interacting with neutral gas; they also note that He II and [O I] are particularly useful when tracing f_{AGN} at low metallicities.

Throughout this work, we have demonstrated that there exists significant confusion in the rest-frame optical line ratio diagnostics when considering only BPASS stellar populations and black hole accretion disk models. The consideration of other sources of ionizing photons, or combinations of those sources, serves to add to the confusion in this parameter space; this indicates that great care should be taken when using these diagrams, beyond what our analysis alone shows.

4.4. Line Ratio Diagnostics at High Redshifts

A complete understanding of line ratio diagnostics requires understanding the coevolution of stars and black holes along with the gas-phase conditions of galaxies across cosmic time. Pre-JWST observations and simulations indicate harder ionizing spectra, increases in ionization parameter, electron density, star formation rate, and decreases in metallicity in predominantly star-forming galaxies out to moderate redshifts (e.g., K. N. Hainline et al. 2009; F. Bian et al. 2010, 2016; B. Siana et al. 2010; L. J. Kewley et al. 2013; P. Madau & M. Dickinson 2014; C. C. Steidel et al. 2014, 2016; R. L. Sanders et al. 2015, 2016, 2018, 2020, 2021; A. E. Shapley et al. 2015, 2019; I. Shvaei et al. 2015, 2018; M. Kaasinen et al. 2017; D. Kashino et al. 2017; A. L. Strom et al. 2017, 2018, 2022; T. L. Suzuki et al. 2017; T. Gburek et al. 2019; R. Maiolino & F. Mannucci 2019; R. C. Simons et al. 2021; B. E. Backhaus et al. 2022; C. Papovich et al. 2022). JWST-era studies have indicated that many of these trends in metallicity, electron temperature, electron density, star formation rates, and ionizing photon production continue out to much higher redshifts (e.g., A. J. Cameron et al. 2023; L. Christensen et al. 2023; M. Curti et al. 2023; S. Fujimoto et al. 2023; K. E. Heintz et al. 2023; Y. Isobe et al. 2023; R. L. Sanders et al. 2023, 2024, 2025; Abdurro'uf et al. 2024; B. E. Backhaus et al. 2024; T. Y.-Y. Hsiao et al. 2024a, 2024b; S. Jain et al. 2025; K. Nakajima et al. 2025); therefore, we find it reasonable to assume that the high-redshift Universe is broadly consistent with lower metallicities and higher ionization parameters.

The evolution of accreting black hole demographics across cosmic time presents another complication to this field. Unfortunately, observations of high-redshift accreting black holes are not necessarily constraining of the physical parameters which drive the ionizing continuum (e.g., black hole mass, spin, accretion rate). Black hole mass estimates (and, by extension, Eddington ratios) are highly uncertain at high redshifts, primarily limited to kinematics of broad permitted lines from a single epoch (e.g., J. E. Greene & L. C. Ho 2005; Y. Harikane et al. 2023; D. D. Kocevski et al. 2023, 2025; V. Kokorev et al. 2023; R. L. Larson et al. 2023; J. Matthee et al. 2024; R. Maiolino et al.

2024; R. E. Hviding et al. 2025; Y. Sun et al. 2025; A. J. Taylor et al. 2025a, 2025b). Unfortunately, less systematics-dominated methods such as reverberation mapping (e.g., R. D. Blandford & C. F. McKee 1982; B. M. Peterson 1993; S. Kaspi et al. 2000; B. M. Peterson et al. 2004) and gas or stellar dynamics (e.g., L. Ferrarese & D. Merritt 2000; K. Gebhardt et al. 2000; J. Kormendy & L. C. Ho 2013) are predominantly not accessible beyond the local Universe with current instrumentation (e.g., F. Pacucci et al. 2023; R. Abuter et al. 2024; M. Golubchik et al. 2024; F. Pacucci & A. Loeb 2024; J. H. Cohn et al. 2025; A. B. Newman et al. 2025).

The [N II]-BPT and VO87 diagrams have been shown to be highly effective at separating star-forming galaxies from accreting supermassive black hole hosts in local studies (e.g., J. A. Baldwin et al. 1981; S. Veilleux & D. E. Osterbrock 1987; G. Kauffmann et al. 2003; L. J. Kewley et al. 2006, 2019; J. R. Trump et al. 2015). However, the local calibrations of these diagnostics may not hold at $z \lesssim 2$ as indicated by pre-JWST studies (e.g., J. A. Baldwin et al. 1981; S. Veilleux & D. E. Osterbrock 1987; L. J. Kewley et al. 2006; S. Juneau et al. 2011, 2014; A. L. Coil et al. 2015), and have been further called into question at $z > 2$ as shown by recent studies with JWST spectroscopy (e.g., A. J. Cameron et al. 2023; R. L. Sanders et al. 2023; H. Übler et al. 2023).

The OHNO diagram has also been used in several works in the early JWST era with observations of very high-redshift galaxies (up to $z \sim 9$; e.g., N. J. Cleri et al. 2023a; D. D. Kocevski et al. 2023; R. L. Larson et al. 2023; J. R. Trump et al. 2023; B. E. Backhaus et al. 2024; A. Calabrò et al. 2024; A. R. Gupta et al. 2024; W. Hu et al. 2024; M. Killi et al. 2024; N. Kumari et al. 2024; F. Arevalo Gonzalez et al. 2025; P. Rinaldi et al. 2025a; J. Scholtz et al. 2025; H. Treiber et al. 2025; P.-F. Wu 2025). Several of these works have noted that nearly all high-redshift observations (particularly at $z \gtrsim 5$) land in the AGN region of the $z \sim 1$ B. E. Backhaus et al. (2022) diagnostic, calling into question the utility of OHNO at early epochs.

Figures 8, 9, and 10 show that the stellar and black hole models are poorly behaved in the [N II]-BPT, VO87, and OHNO diagrams at moderate to high ionization parameters ($\log U \geq -2.75$) and moderate to low metallicities ($Z_{\text{gas}}/Z_{\odot} \leq 0.4$). The OHNO diagram is particularly poorly behaved, with near-complete contamination of the AGN region at high ionization parameters. This indicates that more information beyond these two-dimensional line ratio diagnostics is needed to fully characterize a source at high redshifts where these gas conditions are increasingly common.

5. Summary and Conclusions

In this work, we employ a large photoionization model grid computed using Cloudy to study three optical emission-line ratio diagnostics of ionizing sources: [O III]/ $H\beta$ versus [N II]/ $H\alpha$ (the “[N II]-BPT” diagram; J. A. Baldwin et al. 1981), [O III]/ $H\beta$ versus [S II]/ $H\alpha$ (the “VO87” diagram; S. Veilleux & D. E. Osterbrock 1987), and [O III]/ $H\beta$ versus [Ne III]/[O II] (the “OHNO” diagram; B. E. Backhaus et al. 2022). We analyze the ionizing spectra and the Cloudy models, and perform parameter inference to predict the physical conditions of a source given its optical strong line ratios.

The primary findings of this work are as follows:

1. The optical emission-line ratio diagnostics [N II]-BPT, VO87, and OHNO are strong tracers of the ionization parameter and gas-phase metallicity. At moderate to high ionization parameters ($\log U \geq -2.75$) and moderate to low metallicities ($Z_{\text{gas}}/Z_{\odot} \leq 0.4$), there is significant and sometimes near-complete overlap between the stellar population and black hole accretion disk models (see Figures 8, 9, and 10).
2. We show that the OHNO diagram in particular is most strongly driven by the ionization parameter $\log U$, and is not necessarily sensitive to the physical source of the ionizing photons. The contamination of the AGN region of the OHNO diagram is worse at higher ionization parameters, which makes OHNO a worse diagnostic at increasing redshifts. Thus, we do not recommend the use of OHNO alone as a diagnostic of ionizing sources, particularly in the gas conditions typical of galaxies in the early Universe.
3. There is a significant overlap in the range of the black hole accretion disk and stellar ionizing continua when parameterized by the ratios of the ionizing photon budgets Q in each of the four ionization zones, with the exception of ratios with Q_{veryhigh} (see Figure 2). This is evidence that spectral features which probe >54 eV photons (e.g., He II, [Ne V], etc.) are strong indicators of an ionizing source harder than BPASS stellar populations and should be targets for future study.
4. We show that it is difficult to uniquely constrain the dominant ionizing sources for real observations of high-redshift galaxies with optical strong line ratios alone (see Figure 7).

Our results show that these three optical strong line ratio diagnostics—the [N II]-BPT, VO87, and OHNO diagrams—are highly convenient and useful due to the observability of the rest-frame optical strong lines in many redshift regimes. However, each of the three has underlying biases and confounding behavior which need to be carefully considered for their results to be meaningfully interpreted.

There exist many outstanding questions about the determination of ionizing sources in galaxies at early times. Future works will test these optical diagnostics and many others with large statistical samples, now made accessible with JWST spectroscopy (e.g., N. J. Cleri et al. 2025, in preparation). The impacts of shocks, binary interactions, and other sources of ionization at high redshifts still remain unclear (see Section 4.3.2 for a discussion), and further serve to complicate the task of characterizing high-redshift observations.

Fully understanding the underlying physics that drives the emission from galaxies requires more information than can be obtained from a small number of strong emission-line ratios. While emission-line ratio diagnostics from an integrated spectrum are very convenient tools for providing initial evidence of an ionization mechanism, we need to look beyond using a single piece of information to strictly dichotomize an astrophysical source. The results of this work motivate future observations of high-redshift galaxies with deep spectroscopy from JWST and multiwavelength data from X-ray to radio in order to form a complete picture of the physical mechanisms

driving the ionization conditions of galaxies in the early Universe.

Software: Astropy (Astropy Collaboration et al. 2013), NumPy (C. R. Harris et al. 2020), Matplotlib (J. D. Hunter 2007), Cloudy (G. J. Ferland et al. 2017; C. M. Gunasekera et al. 2023), pandas (J. Reback et al. 2022), XSPEC (K. A. Arnaud 1996).

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The Pennsylvania State University campuses are located on the original homelands of the Erie, Haudenosaunee (Seneca, Cayuga, Onondaga, Oneida, Mohawk, and Tuscarora), Lenape (Delaware Nation, Delaware Tribe, Stockbridge-Munsee), Monongahela, Shawnee (Absentee, Eastern, and Oklahoma), Susquehannock, and Wahzhazhe (Osage) Nations. As a land grant institution, we acknowledge and honor the traditional caretakers of these lands and strive to understand and model their responsible stewardship. We also acknowledge the longer history of these lands and our place in that history.

Author Contributions

N.J.C. led the design and analysis of this work and the proposal from which this work is funded. G.M.O. helped develop the photoionization models used throughout this work. B.E.B., J.L., C.P., and J.R.T. offered high-level directional guidance throughout the work. All other authors provided useful commentary and feedback on the analysis, communication, and interpretation of the results in this work and in the writing of the proposal from which this science is funded, NASA grant No. JWST-AR-05558.

Appendix Line Ratio Diagnostic Animations

In this appendix, we present animated versions (available in the online version of the journal) of the line ratio diagnostics discussed in this work. Figures 11 and 12 show our models on the [N II]-BPT diagram animated in steps of ionization parameter and gas-phase metallicity, respectively. Figures 13 and 14 show our models on the VO87 diagram animated in steps of ionization parameter and gas-phase metallicity, respectively. Figures 15 and 16 show our models on the OHNO diagram animated in steps of ionization parameter and gas-phase metallicity, respectively.

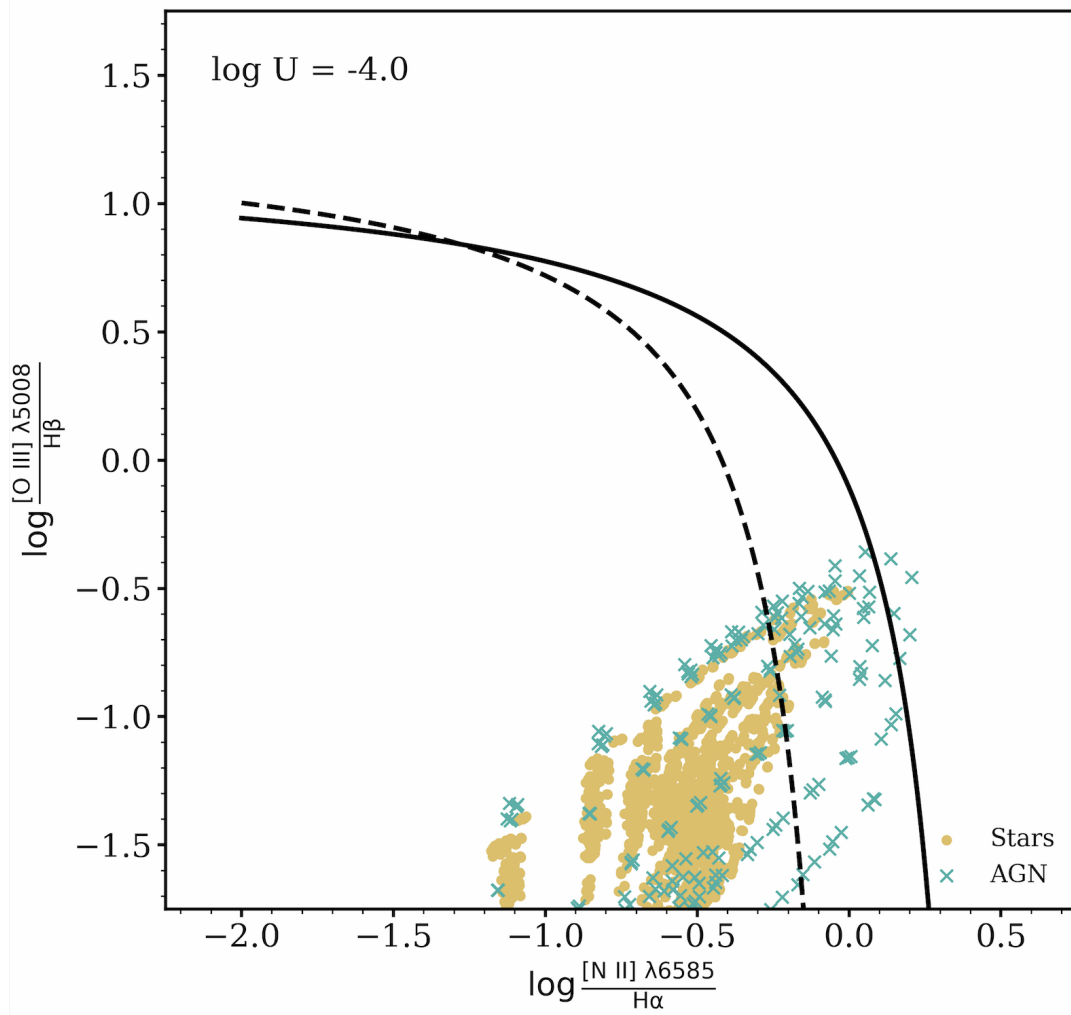


Figure 11. Animation of the [N II]-BPT diagram in steps of ionization parameter, with BPASS stellar population models (gold circles) and black hole accretion disk models (blue crosses) compared against the L. J. Kewley et al. (2001, solid) and G. Kauffmann et al. (2003, dashed) diagnostics. An animation is available showing the change in the ionization parameter from -4 to -1 in 0.25 increments. The real-time duration is 1.9 s. (An animation of this figure is available in the [online article](#).)

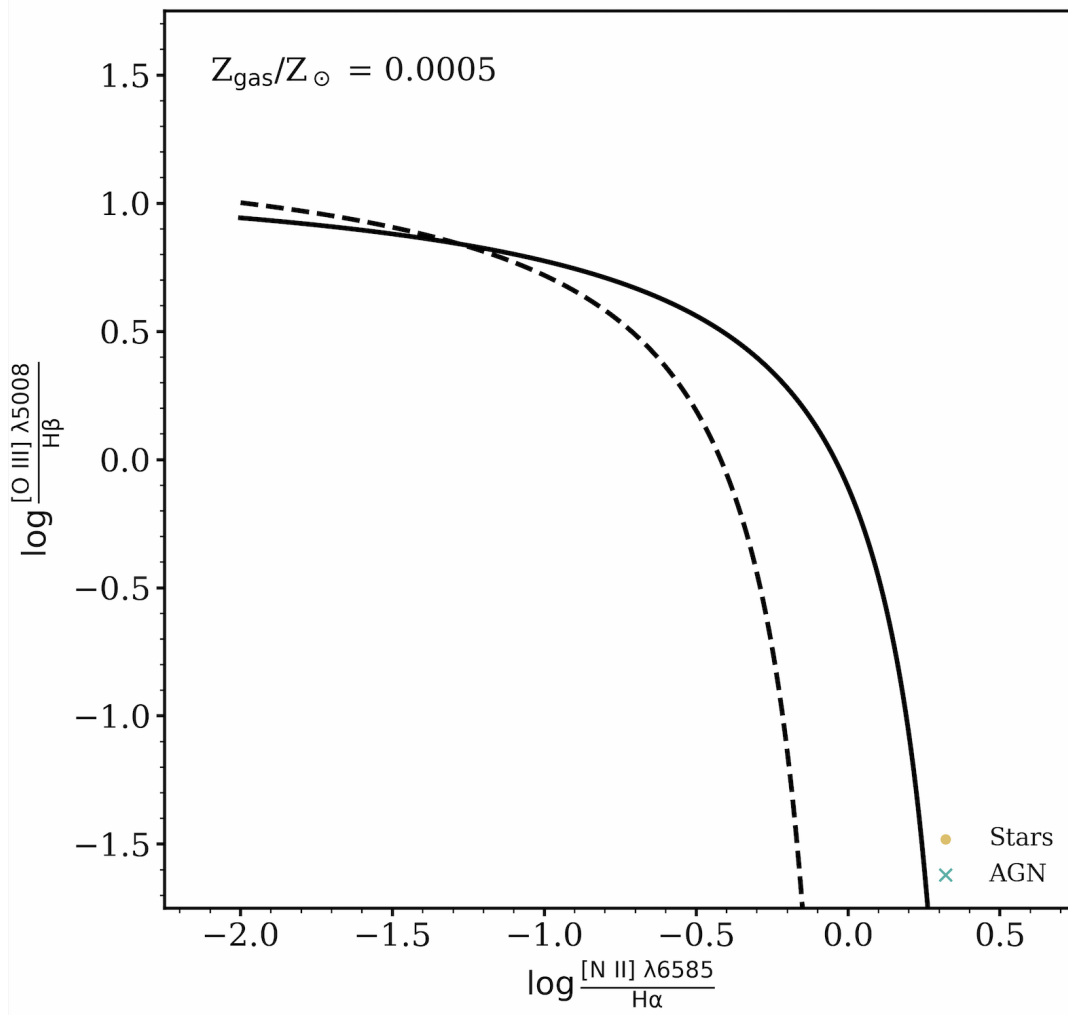


Figure 12. Animation of the [N II]-BPT diagram in steps of gas-phase metallicity, with BPASS stellar population models (gold circles) and black hole accretion disk models (blue crosses) compared against the L. J. Kewley et al. (2001, solid) and G. Kauffmann et al. (2003, dashed) diagnostics. An animation is available showing the change in the gas-phase metallicity from 0.0005 to $2 Z_{\odot}$, in accordance with the grid spacing used in the full model library. The increment steps increase as the animation progresses. The real-time duration is 1.9 s.

(An animation of this figure is available in the [online article](#).)

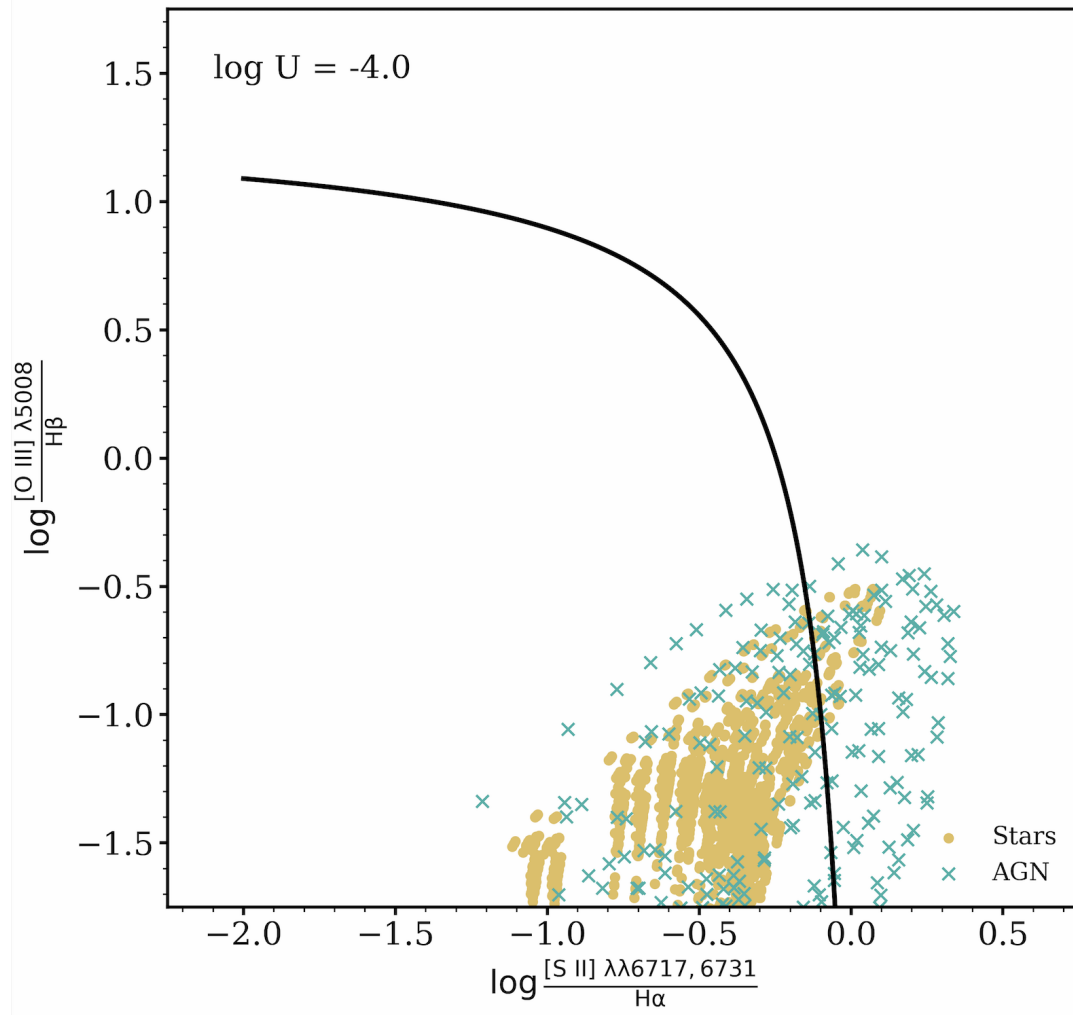


Figure 13. Animation of the VO87 diagram in steps of ionization parameter, with BPASS stellar population models (gold circles) and black hole accretion disk models (blue crosses) compared against the J. R. Trump et al. (2015) diagnostic. An animation is available showing the change in the ionization parameter from -4 to -1 in 0.25 increments. The real-time duration is 1.9 s.
(An animation of this figure is available in the [online article](#).)

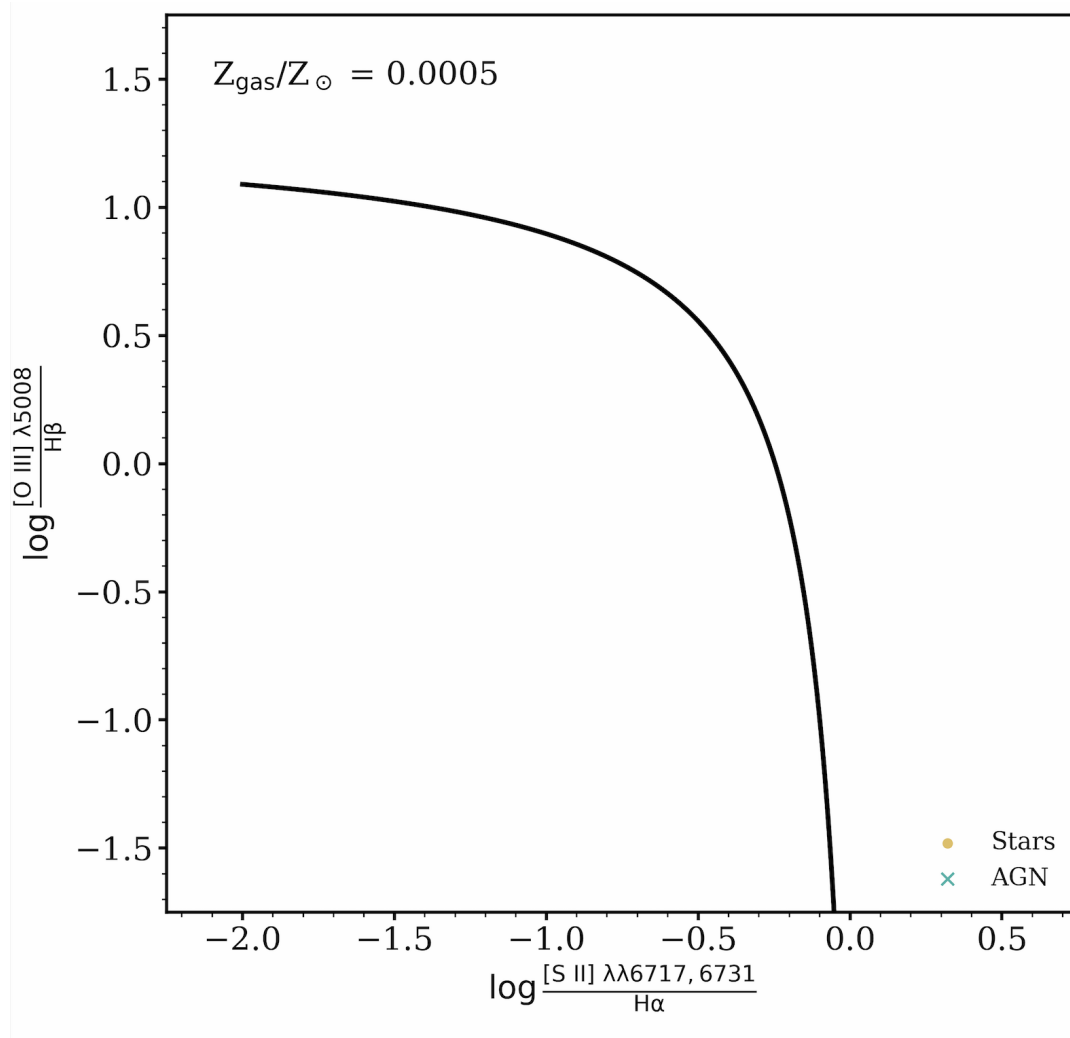


Figure 14. Animation of the VO87 diagram in steps of gas-phase metallicity, with BPASS stellar population models (gold circles) and black hole accretion disk models (blue crosses) compared against the J. R. Trump et al. (2015) diagnostic. An animation is available showing the change in the gas-phase metallicity from 0.0005 to $2 Z_{\odot}$, in accordance with the grid spacing used in the full model library. The increment steps increase as the animation progresses. The real-time duration is 1.9 s.

(An animation of this figure is available in the [online article](#).)

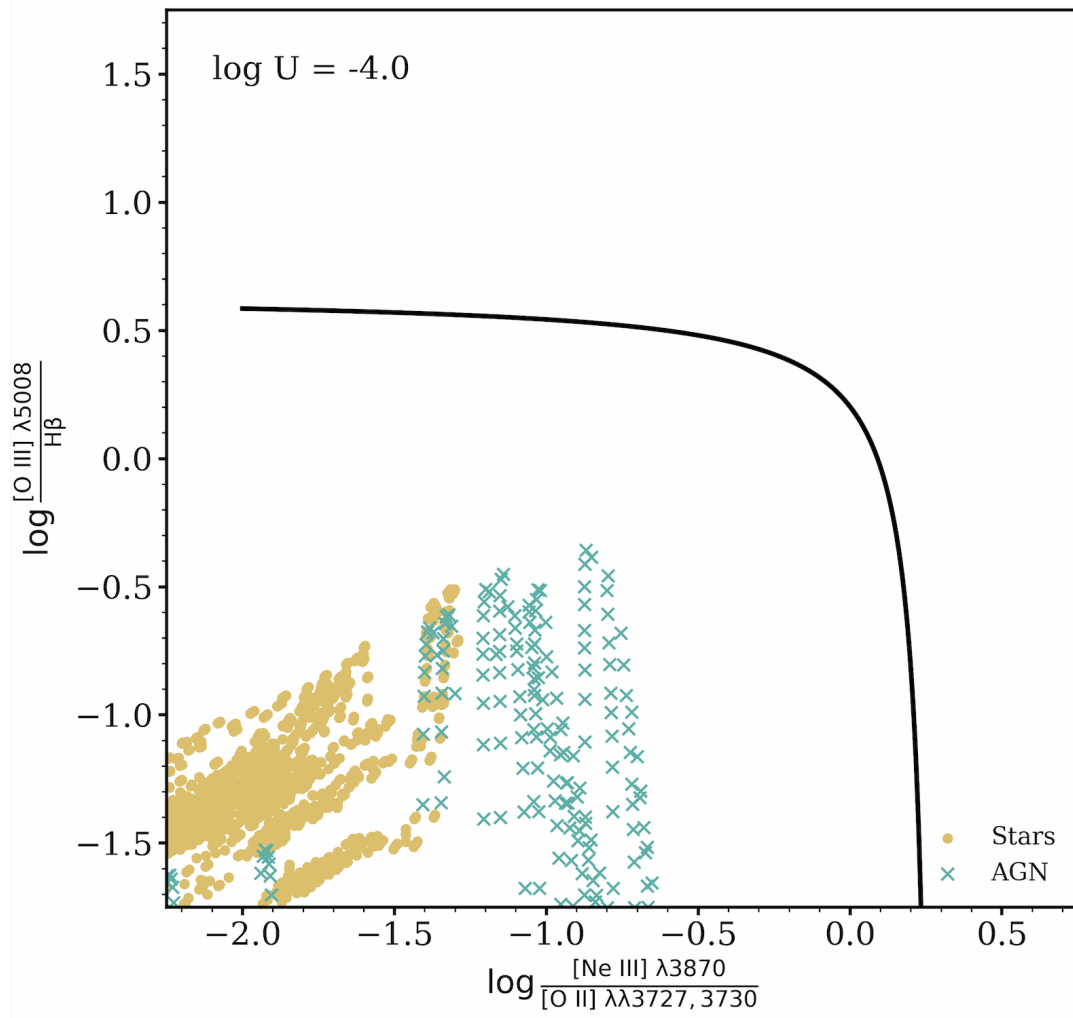


Figure 15. Animation of the OHNO diagram in steps of ionization parameter, with BPASS stellar population models (gold circles) and black hole accretion disk models (blue crosses) compared against the B. E. Backhaus et al. (2022) diagnostic. An animation is available showing the change in the ionization parameter from -4 to -1 in 0.25 increments. The real-time duration is 1.9 s. (An animation of this figure is available in the [online article](#).)

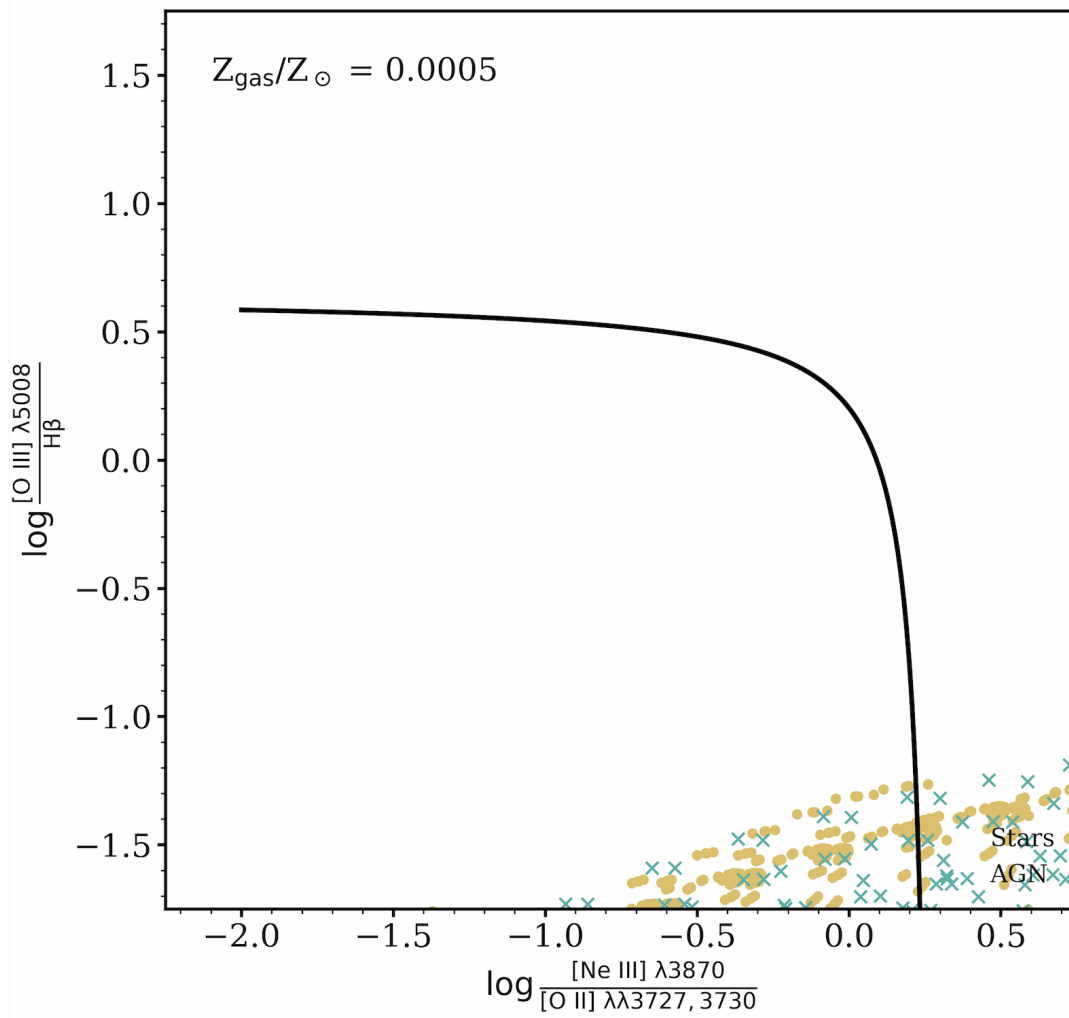


Figure 16. Animation of the OHNO diagram in steps of gas-phase metallicity, with BPASS stellar population models (gold circles) and black hole accretion disk models (blue crosses) compared against the B. E. Backhaus et al. (2022) diagnostic. An animation is available showing the change in the gas-phase metallicity from 0.0005 to $2 Z_{\odot}$, in accordance with the grid spacing used in the full model library. The increment steps increase as the animation progresses. The real-time duration is 1.9 s.

(An animation of this figure is available in the [online article](#).)

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