Supporting Information for:

**Wastewater management strategies for sustained shale gas production**

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S1. Wastewater production data

Historic wastewater production was quantified using biannual waste reports published by the Pennsylvania Department of Environmental Protection (PADEP).¹ Each entry in the data files lists relevant information on the well and operator along with the waste type, quantity, and disposal method selected from a predetermined list established by the PADEP. Because such reporting lagged industry growth in the early stages of Marcellus shale development, complete data began in 2011 and statewide wastewater production reports were available through the end of 2016 and then monthly for 2017 and 2018. Data for each reporting period were filtered to determine the total amount of operator-reported drilling, flowback, and produced fluids generated annually. Flowback and produced fluids were further filtered by disposal method, grouping the PADEP labels that deviate slightly among reporting periods into 5 categories: direct reuse at another frac site; recycling for reuse at another frac site following some level of treatment; treatment at a centralized waste treatment (CWT) facility and subsequent discharge; injection into an underground disposal well; and “other,” which refers to storage or transfer where the end destination is not specified. Note that these data may be inconsistent and incomplete due to variations in operator practices but provide a representative picture of the magnitude of wastewater streams produced in Pennsylvania’s Marcellus region. Total annual wastewater volumes were then predicted by individually forecasting volumes generated during drilling, flowback, and production, as described in the following sections.

S2. Wastewater forecasting: Drilling fluids

From 2011-2018, the annual volume of drilling wastewater has roughly correlated with the number of drilled wells reporting. Given that drilling practices in the Marcellus have been well-established and the data has varied minimally in recent years, an average of 200 m³ of wastewater per well was applied to the number of new wells drilled each year, which were projected from historic trends. SPUD reports from the PADEP were first compiled to determine the number of new wells that commenced drilling in a given year. This number never matched the number of unique new wells reporting drilling fluid waste in the PADEP wastewater reports but approached it (i.e. within 10%) after 2011, presumably as reporting requirements became more robust. Annual drilling rates increased exponentially from 2005-2010 and have fluctuated since peaking in 2011, with rates declining through 2013, rising in 2014, and falling again through 2016 with a decline in natural gas prices (Figure S1). Drilling began to rebound in 2017 and dropped off slightly in 2018, although field-wide natural gas production has continued to rise.

Given the unpredictable array of political, economic, and technical factors governing shale gas production, incorporating a multitude of variables into forecast models would increase complexity without necessarily reducing uncertainty. Since our end goal is simply to demonstrate growing demands for wastewater management and not to pinpoint exact numbers, we developed simplified wastewater forecasts based on natural gas price forecasts. Historic natural gas prices, taken as the average Henry Hub spot price for a given year, are compared with annual drilling rates in Figure S1. There is no direct relationship between the two but declines in drilling generally lag falling natural gas prices by 1 to 4 years.
Figure S1. Trends in the number of wells drilled annually according to PADEP SPUD reports relative to average annual Henry Hub natural gas spot prices from 2005-2018.

We applied the principle of elasticity, which measures how a quantity of supply or demand varies in response to a change in price, to examine the relationship between year-end average natural gas prices ($C_{NG}$) and the number of wells drilled ($N_{SPUD}$) through 2018. This elasticity can be calculated as:

$$E = \frac{\Delta N_{SPUD}}{\Delta C_{NG}}$$  \hspace{1cm} \text{Eqn. (1)}

Historically, natural gas price increases have led to a smaller rise in drilling rates (i.e. more inelastic relationship) relative to the decline in drilling rates resulting from price drops. This discrepancy in responsiveness may be due to the fact that operators can shut down rigs more quickly than they can re-mobilize when markets shift. Because natural gas prices are expected to slowly rise from 2019-2025 according to the World Bank’s latest report (April 2019), a conservative elasticity of 0.5 (the average when gas prices increased steadily from 2012-2014) was applied for projected years. The change in natural gas price in each forecast year was taken as the difference in average prices predicted by the World Bank’s forecast, using the “constant dollar” values that account for inflation. The change in drilling in each future year was calculated by re-arranging Equation 1 with an elasticity of 0.5:

$$\Delta N_{SPUD} = E \times \Delta C_{NG} = 0.5 \Delta C_{NG}$$  \hspace{1cm} \text{Eqn. (2)}

The number of new wells drilled in each forecast year ($n$) was then estimated by multiplying the number of wells drilled in the previous year ($n-1$) by the percent increase in drilling rate, rounding up to the nearest whole well:

$$N_{SPUD,n} = N_{SPUD,n-1}(1 + \Delta N_{SPUD})$$  \hspace{1cm} \text{Eqn. (3)}
These calculations are summarized in Table S1 below. Total annual drilling wastewater volumes were calculated by multiplying the number of wells drilled by the estimated average of 200 m³/well. As previously noted, future drilling rates are influenced by numerous unpredictable external factors and are not directly dependent on natural gas prices, which are also highly uncertain. However, this calculation provides a rough estimate of annual drilling rates barring significant external regulatory or market shifts. Annual drilling activity is expected to continue increasing with rising natural gas prices through 2025, albeit at incremental rates. While drilling declined by 43% from 2014 to 2015 and was down by another 36% in 2016, rates rebounded by 82% in 2017 and are expected to continue rising with improving natural gas prices over the next few years as long as recoverable reserves are accessible. Combined with the 11,789 wells drilled from 2005-2018, our projections result in a cumulative total of 17,199 unconventional wells drilled by the end of 2025, well below Hughes’ conservative estimate of 63,274 total accessible and economically viable wells in the Marcellus region. The projected increase in drilling is also conservative, as there are substantial remaining gas reserves in the Marcellus but we assume rates never recover to the level of the initial 2011-2014 boom.

Table S1. Historic (2011-2018) and projected (2019-2025) natural gas prices and Marcellus drilling rates. Blue entries represent projected values, while black are reported data.

| Year | NG price ($/MMBtu) | % change in NG price | % change in drilling | Elasticity | Wells drilled | Drilling WW (Mm³) |
|------|-------------------|----------------------|---------------------|------------|--------------|------------------|
| 2011 | 4                 | -8.47                | 22.3                | -2.6       | 1956         | 0.40             |
| 2012 | 2.75              | -31.3                | -30.9               | 1.0        | 1352         | 0.32             |
| 2013 | 3.73              | 35.6                 | -10.1               | -0.28      | 1216         | 0.18             |
| 2014 | 4.37              | 17.2                 | 13.0                | 0.76       | 1374         | 0.29             |
| 2015 | 2.62              | -40.1                | -42.9               | 1.1        | 784          | 0.17             |
| 2016 | 2.52              | -3.82                | -35.8               | 9.4        | 503          | 0.06             |
| 2017 | 2.99              | 18.7                 | 82.31               | 4.4        | 917          | 0.16             |
| 2018 | 3.17              | 6.02                 | 3.01                | -2.5       | 778          | 0.16             |
| 2019 | 2.8               | -11.7                | -5.84               | 0.5        | 733          | 0.15             |
| 2020 | 2.9               | 3.57                 | 1.79                | 0.5        | 747          | 0.15             |
| 2021 | 3.0               | 3.45                 | 1.72                | 0.5        | 760          | 0.15             |
| 2022 | 3.1               | 3.33                 | 1.67                | 0.5        | 773          | 0.15             |
| 2023 | 3.2               | 3.23                 | 1.61                | 0.5        | 786          | 0.16             |
| 2024 | 3.3               | 3.12                 | 1.56                | 0.5        | 799          | 0.16             |
| 2025 | 3.4               | 3.03                 | 1.52                | 0.5        | 812          | 0.16             |
S3. Wastewater forecasting: Flowback fluids

Following well completion, mixed gases and fluids flow back to the surface until the produced gas is suitable for treatment and pipeline transport. Initial flowback fluids consist primarily of injected and formation waters with small amounts of entrained gases. Once production begins, gas streams must be continuously separated from smaller and often intermittent volumes of produced fluids consisting primarily of connate brines. Because volumes of flowback and produced fluids associated with gas production are both formation- and well-dependent, we developed forecasts based on the data reported to the PADEP by Marcellus shale gas operators from 2011-2016.\(^1\) In these reports, the flowback period is defined as the first 30 days following the start of production, and all fluids returned thereafter are considered produced fluids.\(^4\) Note that the 2017 reports no longer distinguish between flowback and produced water, the 2017 and 2018 data were not used as a basis for forecasting but are presented as total wastewater volumes in Figure 1 of the manuscript. As validation for the simplified forecast approach developed here, separate flowback volumes in 2017 and 2018 were calculated using the projection approach described below and then added to ‘projected’ produced water volumes for comparison with the total volumes of flowback and produced waters reported to the PADEP (see S4).

Annual flowback and produced volumes were first normalized to the number of unique wells reporting flowback and produced fluids, respectively. Flowback volumes fluctuated from 550-1150 m\(^3\)/well but displayed no temporal trend. Since flowback fluid volumes are not expected to change significantly (barring significant changes in drilling practices) and these historic data are also subject to inconsistencies in operator reporting, an average of 850 m\(^3\) per new well completion was applied in each forecast year. Because flowback fluids are associated with well completion, we based forecasts on the amount of new active wells brought online in a given year. From 2011-2016, the number of new active wells is calculated as the difference between the total number of active and producing wells in successive years from PADEP production reports. This number generally leads the number of wells drilled in a given year as operators address backlogs of early drilled-but-uncompleted (DUC) wells. As of 2016, just over 10,000 wells had been drilled in the Marcellus since 2005 but only 7,690 were both active and producing; the rest are either DUCs or have been plugged or abandoned. The difference between the cumulative number of wells drilled and the total number of active and producing wells in a given year has hovered between ~2400 and 2750 wells since 2011. We assumed that this backlog remains relatively constant at an average of 2600 wells/year as drilling resumes; in reality, the number of wells operators choose to shut in or leave uncompleted rather than bring online will be largely dependent on the economic favorability of production (i.e., natural gas prices and pipeline availability). In each forecast year, we subtracted the 2600 wells that are not producing from the cumulative amount of wells drilled to estimate the total number of active and producing wells.

The number of new wells online in each forecast year, which was assumed to be the number of wells contributing flowback water \((N_{FB})\), was then taken as the difference in the number of active and producing wells between two successive years. Note that this simply equates to the number of wells drilled, which is consistent with the fact that the number of new wells put into production in a given year has generally been at least 99% of the quantity drilled. Total annual flowback volumes were then calculated by multiplying this projected number of new active wells by the assumed average of 850 m\(^3\)/well. These calculations and total flowback wastewater volumes are summarized in Table S2 below.
Table S2. Historic (2011-2016) and projected (2019-2025) flowback wastewater volumes based on new well completions. Blue entries represent projected values while black are reported data. Note that 2017 and 2018 flowback volumes were not distinguished from produced water in the PADEP reports, so these values were calculated based on the projection approach described above and used only as corroboration by comparing the total “projected” flowback and produced volumes for 2017 and 2018 with the actual values reported to PADEP.

| Year | Cumulative wells drilled | Active + producing wells | Drilled, not producing | New wells online | Flowback WW (Mm³) |
|------|--------------------------|--------------------------|------------------------|------------------|------------------|
| 2011 | 4865                     | 2218                     | 2647                   | 1004             | 1.30             |
| 2012 | 6217                     | 3557                     | 2660                   | 1339             | 1.55             |
| 2013 | 7433                     | 4912                     | 2521                   | 1355             | 0.95             |
| 2014 | 8807                     | 6043                     | 2764                   | 1131             | 1.99             |
| 2015 | 9591                     | 6924                     | 2667                   | 881              | 1.15             |
| 2016 | 10094                    | 7690                     | 2404                   | 766              | 0.54             |
| 2017 | 11011                    | 8411                     | 2600                   | 721              | 0.61             |
| 2018 | 11789                    | 9189                     | 2600                   | 778              | 0.66             |
| 2019 | 12522                    | 9922                     | 2600                   | 733              | 0.62             |
| 2020 | 13269                    | 10699                    | 2600                   | 747              | 0.63             |
| 2021 | 14029                    | 11429                    | 2600                   | 760              | 0.65             |
| 2022 | 14802                    | 12202                    | 2600                   | 773              | 0.66             |
| 2023 | 15588                    | 12988                    | 2600                   | 786              | 0.67             |
| 2024 | 16387                    | 13787                    | 2600                   | 799              | 0.68             |
| 2025 | 17199                    | 14599                    | 2600                   | 812              | 0.69             |
S4. Wastewater forecasting: Produced fluids

Similar to flowback, normalized produced fluid volumes also varied inconsistently from 500-1050 m$^3$/well. An average of 750 m$^3$/well was applied to the projected numbers of active and producing wells calculated in Section 1.3 to estimate total volumes of produced wastewater from 2017-2025. These data are summarized in Table S3, along with the total annual historic and projected wastewater volumes summed from drilling, flowback, and produced waters (which are plotted in Figure 1 of the manuscript). Note that the increase in total wastewater production from 2015-2016 despite a sharp decline in drilling was largely due to an increase in the volume of produced water per reporting well, from 725 m$^3$/well in 2015 to 1140 m$^3$/well in 2016. As mentioned in S3, this simplified approach for individually projecting flowback and produced waters was corroborated by comparing our values to the single volume including flowback and produced water reported to PADEP for 2017 and 2018. In both years our calculated values are within 10% of the actual values.

Table S3. Historic (2011-2016) and projected (2019-2025) produced wastewater volumes based on field-wide quantities of active and producing wells. Blue entries represent projected values while black are reported data. Distinct produced water data was not available for 2017 and 2018 so wastewater volumes in these years were also “projected” using the approach described above and added to projected flowback volumes (Table S4) for corroboration with the reported totals of flowback and produced waters in 2017 and 2018.

| Year | Active + producing wells | Produced WW (Mm$^3$) | Total WW (Mm$^3$) |
|------|--------------------------|----------------------|-------------------|
| 2011 | 2218                     | 1.51                 | 3.21              |
| 2012 | 3557                     | 2.68                 | 4.54              |
| 2013 | 4912                     | 2.52                 | 3.65              |
| 2014 | 6043                     | 4.61                 | 6.89              |
| 2015 | 6924                     | 4.89                 | 6.20              |
| 2016 | 7690                     | 6.11                 | 6.72              |
| 2017 | 8411                     | 6.31                 | 7.08              |
| 2018 | 9189                     | 6.89                 | 7.72              |
| 2019 | 9922                     | 7.44                 | 8.21              |
| 2020 | 10699                    | 8.00                 | 8.79              |
| 2021 | 11429                    | 8.57                 | 9.37              |
| 2022 | 12202                    | 9.15                 | 9.96              |
| 2023 | 12988                    | 9.74                 | 10.6              |
| 2024 | 13787                    | 10.3                 | 11.1              |
| 2025 | 14599                    | 11.0                 | 11.8              |
S5. Wastewater disposal practices

As noted in Section 1.1, wastewater volumes reported to the PADEP were also filtered by disposal practice: reuse; recycling following some level of treatment at a CWT or residual waste processing facility; treatment at a centralized facility and subsequent discharge; injection; and “other.” Disposal at publically owned treatment facilities, which are typically not equipped to treat oil and gas waste, voluntarily ceased in 2011 following government requests and has been formally prohibited by a 2016 EPA rule. Figure 1b in the manuscript summarizes trends in wastewater disposal practices from 2011-2018; full data for 2019 were not available at the time of writing. Reuse refers to direct reuse at another well site, whereas recycling involves treatment at a centralized facility prior to reuse. Centralized waste treatment (CWT) facilities are specifically designed to treat industrial wastewater and hold NPDES permits for post-treatment discharge. Injection in designated brine disposal wells is regulated by the EPA’s Underground Injection Control (UIC) Program. Because Pennsylvania only has 8 such wells, many of which do not currently accept Marcellus wastewater or are privately owned and operated, injection typically occurs in Ohio. In Figure 1b, “other” accounts for wastewater held in storage (typically with on-site surface impoundments) or sent to transfer facilities, presumably for subsequent recycling or reuse.

S6. Mapping wastewater disposal pathways

Current Marcellus shale gas production wells and wastewater treatment or injection sites were mapped using ArcGIS v10.4 to estimate transport costs for the economic analysis and visualize the current accessibility of each disposal option. Figure 2 of the manuscript illustrates both the spatial distribution and relative capacities of available disposal sites. Only treatment facilities that are currently equipped and permitted to receive wastewater from Marcellus shale gas operations and operational injection wells were included in the analysis of current treatment options, as described below.

The biannual PADEP wastewater reports were used to identify centralized treatment facilities that treat and discharge Marcellus wastewaters. An updated list of all waste facilities in the operator reporting system obtained from the PADEP was then used to identify which facilities currently hold NPDES permits. These lists were refined to determine which plants are currently operational and able to treat fracking wastewater. In cases where permits only specified waste streams from other industrial operations (e.g. coalbed methane connate), it was confirmed by phone that wastewaters from the oil and gas industry are not accepted. Geospatial locations of the few CWT facilities that do currently treat and discharge Marcellus wastewaters to the environment were pulled from the PADEP data for mapping. Facility capacities were taken as the design flows listed in their NPDES permits or from information provided by the company. The PA brine disposal wells were matched with capacities reported by the EPA and geospatial coordinates were obtained from the PADEP oil and gas mapping database. Locations of Ohio disposal wells were obtained from the Ohio Department of Natural Resources (DNR). Because disposal is regulated by the maximum allowable injection pressure rather than the amount of brine injected, well capacities were taken as the average injection rate from 2010-2015.
As discussed in the manuscript, we compared existing disposal options with dedicated large-scale injection into depleted oil wells. While wastewater could also potentially be reused in waterfloods to enhance oil recovery from mature active wells, most existing oil operations currently recycle water within the field and supplement with produced waters on site, significantly reducing or eliminating the need to purchase external makeup water. An increased supply of fracking wastewater could promote expanded use of waterflooding in aging fields, but this option was not considered here given the lack of data on when and where waterflooding could be applicable and the fact that recycling produced fluids in the field would likely be cheaper than transporting produced fluids from fracking. Orphaned wells, which were abandoned prior to 1985 and have not affected nor benefited current property owners, were also excluded due to a greater likelihood that well location or quality would prohibit conversion to an injection well. Wells classified as ‘DEP abandoned’, which have ceased production but have been inspected by the DEP and can be plugged at the DEP’s discretion, and ‘DEP plugged’, which refers to depleted wells that have been plugged by the DEP, were considered as prospective wastewater repositories. Wells in these categories have been subjected to some level of regulatory oversight and are likely better suited to repurpose as injection wells.

A list of plugged and abandoned wells downloaded from the PADEP’s oil and gas reporting site was filtered to include only oil wells and the coordinates of the resulting 3,564 wells were used in GIS mapping. To facilitate calculation of transport distances and account for the fact that many individual wells will not be geologically or geographically suitable for wastewater storage, five oil well “hubs” were designated as wastewater receiving points. A commercialized wastewater injection system would likely follow a similar framework whereby central disposal well operators would maintain groups of close-proximity wellheads to optimize efficiency. While the hub allocation applied here is an oversimplification, it suffices to estimate the accessibility of depleted oil wells in each region considering that the exact number and location of suitable wells will require extensive site characterization and regulatory review.

To compare the proximity of treatment options to sources of wastewater generation, locations of unique and active shale gas wells were filtered from the 2015 PADEP production data. We accounted for the fact that best practices differ between the two production hotspots in the Northeast and Southwest by dividing wells into these regions for separate analyses. While linking wastewaters produced by each well to capacities of available disposal options would provide more robust estimates, this approach is sufficient for comparing relative costs of each disposal option within the scope of this work.

S7. Disposal cost estimates

A high-level economic analysis was performed to compare the operational costs of prospective options to handle projected wastewater volumes, namely centralized waste treatment and discharge; injection in OH disposal wells; and injection in depleted PA oil wells. Injection in the few existing PA brine disposal wells was omitted from the cost analysis because existing dedicated wells accept little wastewater from the Marcellus. For each option, only the operational costs of transport and disposal were considered. While permitting and equipping the depleted wells for injection would elicit upfront costs, accommodating
projected wastewater generation in lieu of this option will require constructing new dedicated treatment facilities and/or siting and drilling new disposal wells, both of which involve significant capital investments. In light of the limited data available on the costs of permitting, designing, and constructing these facilities, capital costs are excluded from this analysis. For consistency, all costs taken from literature were scaled to 2017 USD.

Transport distances from wellheads to disposal sites were first estimated using the ArcGIS Network Analyst extension, assuming wastewater is trucked from frac sites to disposal destinations per current industry practices. Specifically, we ran “closest facility” analyses, which compute the shortest roadway distance between input starting points and potential destinations, between the active wellheads in each region (i.e. Northeast and Southwest) and each set of disposal facilities (CWT, OH injection wells, and PA depleted oil wells). Because the range in distances was often significant given the wide geographic distribution of wells and disposal sites, the 5th percentile, mean, and 95th percentile of these distances were used to calculate low, “average,” and high transport costs, respectively. For direct reuse or recycling, a range of 5-9 miles between successive wellheads is assumed.

A fixed cost of $0.04/bbl/mi was then applied to estimate the range in costs associated with trucking wastewater to disposal sites. Network analyses created for depleted oil well hubs in each region are provided as an example in Figure S2.

Figure S2. GIS network analysis between active production wells and depleted PA oil well “hubs.”

The costs of treatment or disposal at each class of facility were then estimated based on reported data. For reuse or recycling without pre-treatment at a centralized facility, costs were assumed to range from $0/bbl in the case of direct reuse to $1-$3.50/bbl for minimal on-site treatment. Treatment costs at dedicated CWT facilities will vary based on wastewater quality, effluent quality standards, and treatment processes. According to industry representatives, removing TDS via distillation cost $6.35-$8.50/bbl in 2011, within the range of $0.12-$0.25/gal ($5.04-$10.50/bbl) estimated by the PADEP for various treatment techniques. The PADEP estimates were used to bound the range of treatment costs at CWT facilities. Injection costs at the wellhead are assumed to range from $3-$5, but for OH wells we also account for the $0.20 surcharge that is currently levied on out-of-state waste disposal. Operational cost breakdowns for all disposal pathways are illustrated in Figure 3 of the manuscript and summarized in Table S4 below.
Table S4. Marcellus wastewater transport and treatment costs by region.

| Cost                        | Northeast PA |          | Southwest PA |          |
|-----------------------------|--------------|----------|--------------|----------|
|                             | Low         | ‘Likely’ | High         | Low      | ‘Likely’ | High         |
| **Reuse/recycling**         |              |          |              |          |          |              |
| Transport distance (mi)     | 5           | 7        | 9            | 5        | 7        | 9            |
| Transport cost ($/bbl)      | $0.21       | $0.30    | $0.39        | $0.21    | $0.30    | $0.39        |
| Treatment cost ($/bbl)      | $0.00       | $1.00    | $3.50        | $0.00    | $1.00    | $3.50        |
| Total disposal cost ($/bbl) | $0.21       | $1.37    | $4.13        | $0.21    | $1.37    | $4.13        |
| **Centralized waste treatment** |          |          |              |          |          |              |
| Transport distance (mi)     | 6.88        | 24.1     | 50.4         | 7.82     | 26.9     | 43.3         |
| Transport cost ($/bbl)      | $0.29       | $1.03    | $2.16        | $0.33    | $1.15    | $1.85        |
| Treatment cost ($/bbl)      | $5.39       | $8.31    | $11.24       | $5.39    | $8.31    | $11.24       |
| Total disposal cost ($/bbl) | $5.69       | $9.35    | $13.39       | $5.73    | $9.47    | $13.09       |
| **Injection in OH brine disposal well** |          |          |              |          |          |              |
| Transport distance (mi)     | 148         | 250      | 320          | 46       | 70       | 101          |
| Transport cost ($/bbl)      | $6.33       | $10.70   | $13.70       | $1.97    | $3.00    | $4.32        |
| Injection cost ($/bbl)      | $3.00       | $4.00    | $5.00        | $3.00    | $4.00    | $5.00        |
| Out-of-state fee ($/bbl)    | $0.20       | $0.20    | $0.20        | $0.20    | $0.20    | $0.20        |
| Total disposal cost ($/bbl) | $9.53       | $14.90   | $18.90       | $5.17    | $7.20    | $9.52        |
| **Injection in PA depleted oil well** |          |          |              |          |          |              |
| Transport distance (mi)     | 66.5        | 135      | 198          | 12.58    | 45.51    | 69.73        |
| Transport cost ($/bbl)      | $2.85       | $5.78    | $8.47        | $0.54    | $1.95    | $2.98        |
| Injection cost ($/bbl)      | $3.00       | $4.00    | $5.00        | $3.00    | $4.00    | $5.00        |
| Total disposal cost ($/bbl) | $5.85       | $9.78    | $13.47       | $3.54    | $5.95    | $7.98        |
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