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SHASTA
Subsurface Hydrogen Assessment, Storage, and Technology Acceleration

SHASTA-HELP
Hydrogen Estimator for Logistical Planning Tool

Subsurface Hydrogen Assessment, Storage, and Technology Acceleration (SHASTA) - Hydrogen Estimator for Logistical Planning (HELP) User's Manual

November 2023

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NATIONAL ENERGY TECHNOLOGY LABORATORY
Pacific Northwest NATIONAL LABORATORY
Lawrence Livermore National Laboratory
Sandia National Laboratories

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Subsurface Hydrogen Assessment, Storage, and Technology Acceleration - Hydrogen Estimator for Logistical Planning (SHASTA-HELP) User's Manual

November 2023

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Abstract

This user's manual describes version 1.0 of the SHASTA-HELP (Subsurface Hydrogen Assessment, Storage, and Technology Acceleration (SHASTA) - Hydrogen Estimator for Logistical Planning (HELP)) tool and provides instructions for use. The purpose of the SHASTA-HELP tool is to integrate the suite of tools developed by the SHASTA research team in a web-based framework for ease of access and more advanced, integrated analysis. This tool contains functionality for estimating the storage potential of pure and blended natural gas-hydrogen mixtures in various subsurface formations and is intended to be used for pre-characterization or site screening purposes. Detailed storage analysis should be conducted by full reservoir simulation models.

Acknowledgments

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Acronyms and Abbreviations

CH_4	Methane
DOE	U.S. Department of Energy
EIA	U.S. Energy Information Administration
H_2	Hydrogen
GUI	Graphical User Interface
LLNL	Lawrence Livermore National Laboratory
NETL	National Energy Technology Laboratory
PNNL	Pacific Northwest National Laboratory
SNL	Sandia National Laboratory
SHASTA	Subsurface Hydrogen Assessment, Storage, and Technology Acceleration
SHASTA-HELP	Hydrogen Estimator for Logistical Planning
STP	Standard temperature and pressure
UGS	Underground gas storage

Contents

Figures

1.0 Introduction

SHASTA is a research collaboration between four U.S. Department of Energy (DOE) National Laboratories including the National Energy Technology Laboratory (NETL), Pacific Northwest National Laboratory (PNNL), Lawrence Livermore National Laboratory (LLNL), and Sandia National Laboratory (SNL), focused on determining the technical feasibility of hydrogen storage in subsurface systems and quantifying the associated operational risks. The purpose of the SHASTA-HELP tool is to integrate the suite of tools developed by the SHASTA research team in a web-based framework for ease of access and more advanced, integrated analysis.

SHASTA-HELP 1.0 contains functionality for estimating the storage potential of pure and blended natural gas-hydrogen mixtures in various subsurface formations including natural gas storage sites, depleted gas fields, saline aquifers, and salt caverns. The tool relies on a volumetric approach, accepts a variety of inputs, and is intended to be used for characterization or site screening purposes only. Detailed storage analysis should be conducted by full reservoir simulation models. More information on methods to estimate hydrogen storage can be found in these references: Lackey et al. (2023), Mouli-Castillo et al. (2021), Chen et al. (2023), and Lankof and Tarkowski (2020).

This edition of the user manual describes the storage potential functionality in SHASTA-HELP.

Future versions of SHASTA-HELP will include functionality to:

- Rapidly assess hydrogen storage and delivery (including transient evolution and steady-state operations) in a variety of reservoirs.
- Perform techno-economic analyses for the construction of new subsurface hydrogen storage facilities or the conversion of existing facilities.
- Characterize storage potential amidst geologic uncertainty and assess the sensitivity of storage volumes to uncertain parameters.
- Facilitate the sharing of public or SHASTA-generated datasets.
- Interact with spatial (i.e., map-based) displays of tool outputs.

2.0 Equations and Methods Used for Working Gas Energy Calculations for Existing U.S. Underground Storage Facilities

The working gas energy of hydrogen (H_2) that can be stored in existing U.S. underground gas storage (UGS) facilities, $WGE_{H_{2,a}}$, is calculated using Equation (1):

$$WGE_{H_{2,a}} = LHV_{H_2}\rho_{H_2,r}\left(\frac{\rho_{CH_4,a}}{\rho_{CH_4,r}}\right)WGV_{CH_{4,a}} \tag{1}$$

where LHV_{H_2} is the lower heating value of H_2, $\rho_{H_2,r}$ is the density of H_2 in the storage reservoir at storage conditions when the reservoir is full, $\rho_{CH_4,a}$ is the density of methane (CH_4) at the ground surface conditions specified (101.56 kPa and 15.56 ˚C), $\rho_{CH_4,r}$ is the density of CH_4 in the storage reservoir at storage conditions when the reservoir is full, and $WGV_{CH_{4,a}}$ is the working gas volume of CH_4 reported at the ground surface conditions at 101.56 kPa and 15.56 ˚C.

The working gas volume of H_2, $WGV_{H_{2,a}}$ that can be stored in a UGS reservoir is calculated as:

$$WGV_{H_{2,a}} = \left(\frac{\rho_{H_2,r}}{\rho_{H_2,a}}\right)\left(\frac{\rho_{CH_4,a}}{\rho_{CH_4,r}}\right)WGV_{CH4,a}, \tag{2}$$

where $\rho_{H_2,a}$ is the density of hydrogen at 101.56 kPa and 15.56 ˚C.

The working gas energy of blended H_2-CH_4 mixtures, WGE_{mix}, is calculated using

$$WGE_{mix} = LHV_{H_2}\rho_{H_2,r}\left[VF_{H_2,r}\left(\frac{\rho_{CH_4,a}}{\rho_{CH_4,r}}\right)WGV_{CH4,a,mix}\right] + LHV_{CH_4}\rho_{CH_4,r}\left[VF_{CH_4,r}\left(\frac{\rho_{CH_4,a}}{\rho_{CH_4,r}}\right)WGV_{CH4,a,mix}\right], \tag{3}$$

where $VF_{H_2,r}$ is the volume fraction of H_2 in the mixture at storage conditions when the reservoir is full, $VF_{CH_4,r}$ is the volume fraction of CH_4 in the mixture at storage conditions when the reservoir is full, and LHV_{CH_4} is the lower heating value of CH_4. $VF_{H2,r}$ was calculated using

$$VF_{H_2,r} = \frac{\frac{\rho_{H_2,a}}{\rho_{H_2,r}}VF_{H_2,a}}{\frac{\rho_{H_2,a}}{\rho_{H_2,r}}VF_{H_2,a} + \frac{\rho_{CH_4,a}}{\rho_{CH_4,r}}VF_{CH_4,a}}, \tag{4}$$

where $VF_{H_2,a}$ is the volume fraction of H_2 in the mixture at the surface temperature and pressure (101.56 kPa and 15.56 ˚C), $VF_{CH_4,a}$ is the volume fraction of CH_4 in the mixture at surface conditions, $\rho_{H_2,a}$ is the density of H_2 at surface conditions, and $\rho_{CH_4,a}$ is the density of CH_4 at surface conditions. In Equation (3),

$VF_{CH4,r} = 1 - VF_{H_2,r}$. The working gas volumes of H_2, $WGV_{H2,mix}$, and CH_4, $WGV_{CH4,mix}$, in blended H_2-CH_4 mixtures were calculated with their respective density ratio:

$$WGV_{H_2,mix} = \left(\frac{\rho_{H_2,r}}{\rho_{H_2,a}}\right) VF_{H_2,r} \left(\frac{\rho_{CH_4,a}}{\rho_{CH_4,r}}\right) WGV_{CH4,a} \quad (5)$$

$$WGV_{CH_4,mix} = VF_{CH_4,r} \left(\frac{\rho_{CH_4,a}}{\rho_{CH_4,r}}\right) WGV_{CH4,a}. \quad (6)$$

Table F1 in Appendix F provides definitions for all terms described in Equations (1)–(6). An application of this method and equations to assess existing natural storage reservoirs across the United States to estimate the amount of H_2 that could be potentially stored underground, either as a pure gas or mixed with natural gas, can be found in Lackey et al. (2023).

3.0 Initiating SHASTA-HELP

The web-based version of the tool can be accessed here: https://shasta-help.pnnl.gov. There is also a downloadable version of the tool that is publicly available on GitHub and can be found here: https://github.com/netl-ric/wgv_calculation. More details about the downloadable version of the tool are included in Appendix G.

Figure 3.1 shows the main page of the SHASTA-HELP web-based tool. The "Map" tab at the top is still under development. Under the "Calculation" tab at the top, there are two main options:

- AN EXISTING NATURAL GAS STORAGE FACILITY
  - ➢ Appropriate for all natural gas storage facilities with a known working gas volume regardless of reservoir type.

- A PROSPECTIVE GEOLOGIC FORMATION
  - ➢ Appropriate for a geologic formation (depleted gas field, saline aquifer, or salt cavern) with unknown working gas volume.

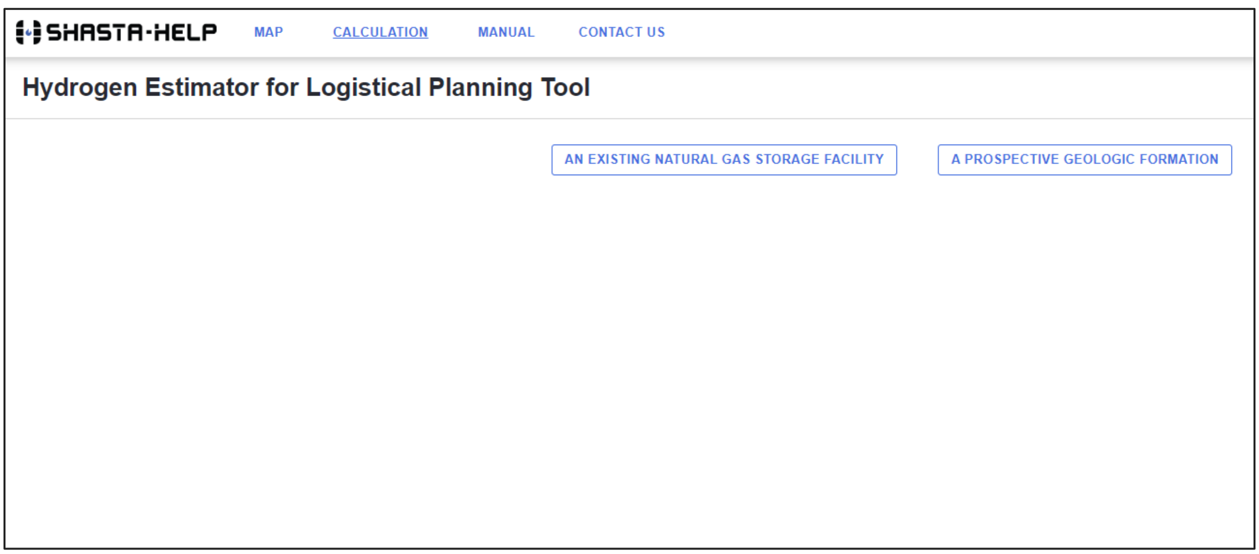

Figure 3.1: The main page (Calculation tab) of SHASTA-HELP web-based tool.

4.0 Running the Tool

AN EXISTING NATURAL GAS STORAGE FACILITY:

If "An Existing Natural Gas Storage Facility" is selected on the main page, a new page will be displayed as shown in Figure 4.1. You can always go back to the main page by clicking on "BACK TO STORAGE TYPE SELECTION" button. The "Units" radio button provides the option to enter the input values and generate the results in either SI or Imperial units. Switching the radio button will change the units of both input and output values. Input parameters on the left-side of the page are auto populated with default values; however, the user is encouraged to modify these values. The definitions of parameters are included in the page at the bottom right. Once input parameters are finalized with default or modified values (all entries must contain a value), press the "RUN CALCULATION" button and the results will appear at the top right of the page. The results include the working gas mass, working gas volume, and working gas energy of hydrogen, methane, and total blend. To test new input parameters, simply modify the parameters and press "RUN CALCULATION" again. For convenience, the results can be exported by clicking on the "EXPORT TO CSV" button under the results table. Also, under the results table, the output values can be set to be displayed in scientific or standard notation with varying precision.

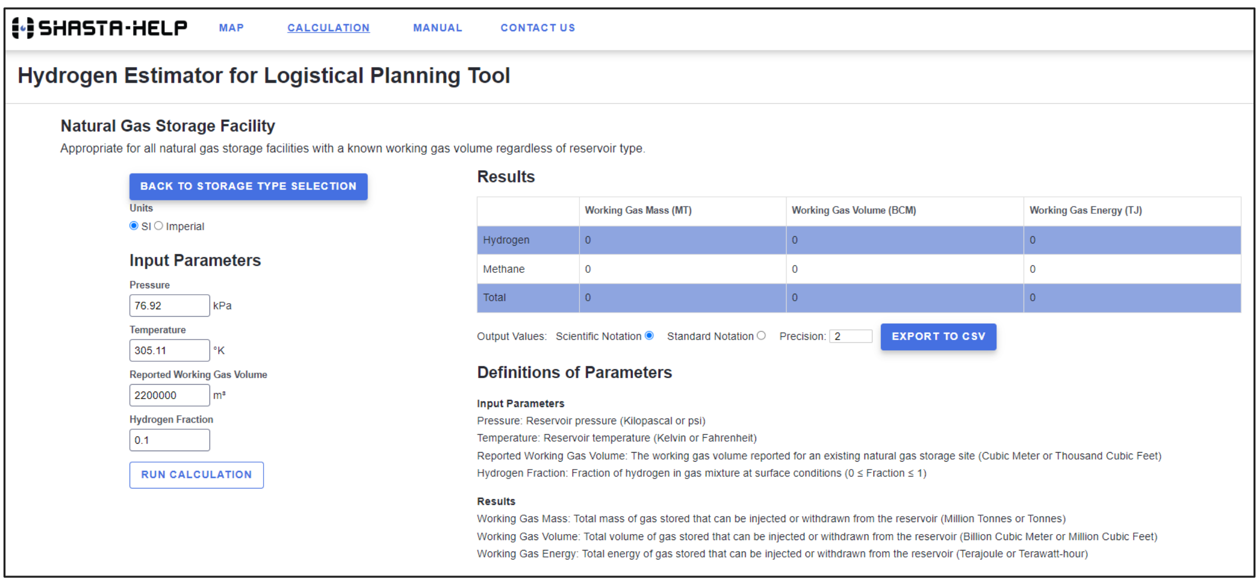

Figure 4.1: "Natural Gas Storage Facility" page of SHASTA-HELP web-based tool.

A PROSPECTIVE GEOLOGIC FORMATION:

If "A Prospective Geologic Formation" is selected on the main page, three options will appear as shown in Figure 4.2:

- DEPLETED GAS FIELD
- SALINE AQUIFER
- SALT CAVERN

Each type of formation is associated with different set of input parameters and calculations.

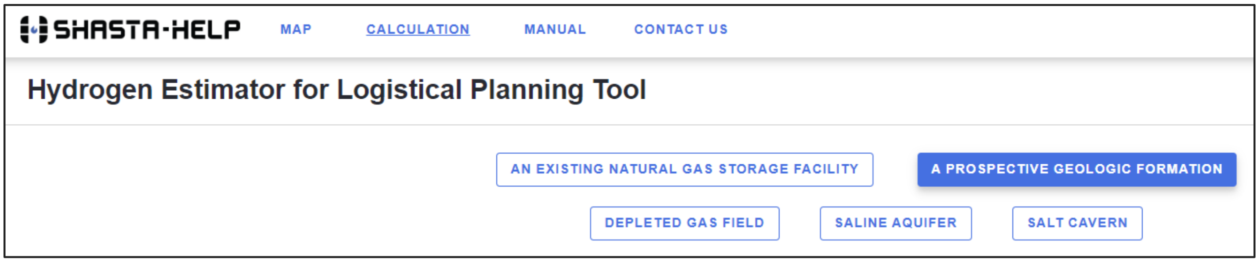

Figure 4.2: Geologic formation options under "A Prospective Geologic Formation" category.

DEPLETED GAS FIELD

If "Depleted Gas Field" is selected under "A Prospective Geologic Formation," two more options will appear as shown in Figure 4.3, based on whether the cumulative gas production is available or not:

- KNOWN CUMULATIVE GAS PRODUCTION
- UNKNOWN CUMULATIVE GAS PRODUCTION

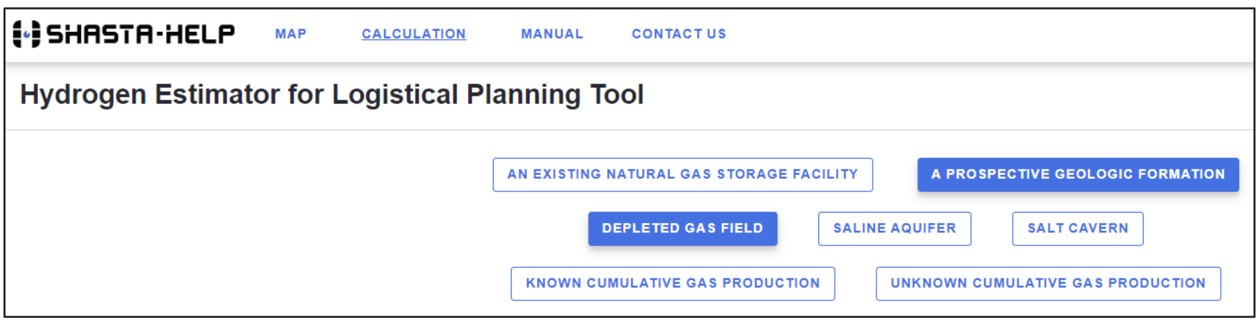

Figure 4.3: Options under "Depleted Gas Field" category, based on availability of cumulative gas production.

KNOWN CUMULATIVE GAS PRODUCTION

If "Known Cumulative Gas Production" is selected under "Depleted Gas Field," a new page will be displayed as shown in Figure 4.4 for calculations related to depleted gas fields, when cumulative gas production is known. The functionality of the unit radio button, input parameters, run button, and results table are as described before.

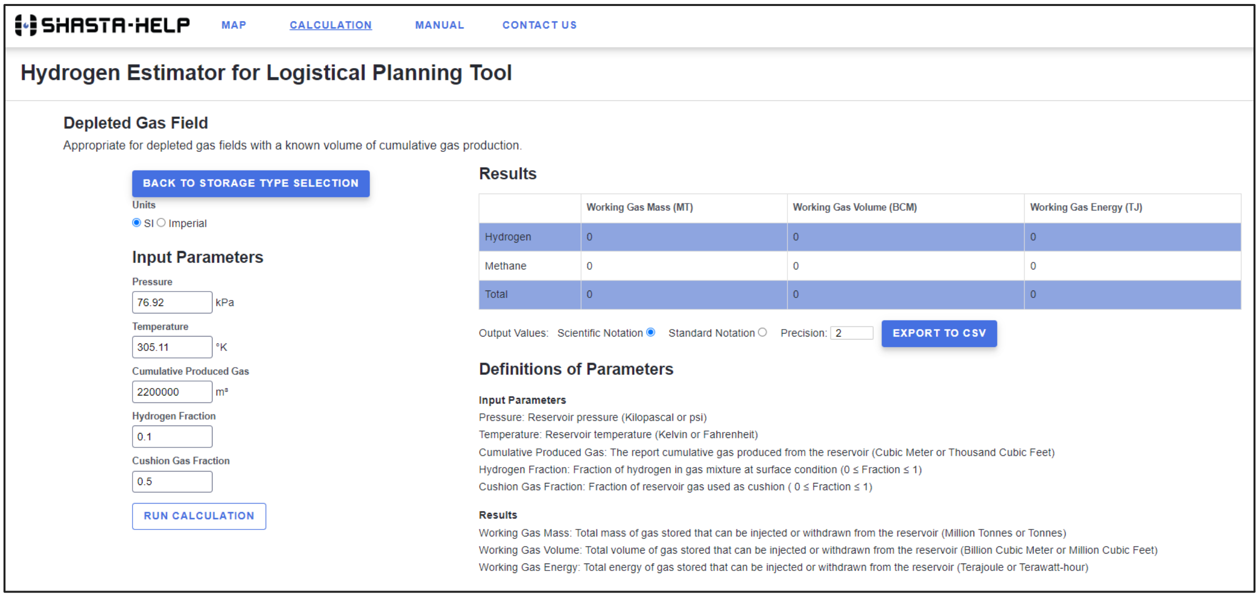

Figure 4.4: "Depleted Gas Field" page of SHASTA-HELP web-based tool when the cumulative gas production is known.

UNKNOWN CUMULATIVE GAS PRODUCTION

If "Unknown Cumulative Gas Production" is selected under "Depleted Gas Field," a new page will be displayed as shown in Figure 4.5 for calculations related to depleted gas fields, when cumulative gas production is unknown. The functionality of the unit radio button, input parameters, run button, and results table are as described before.

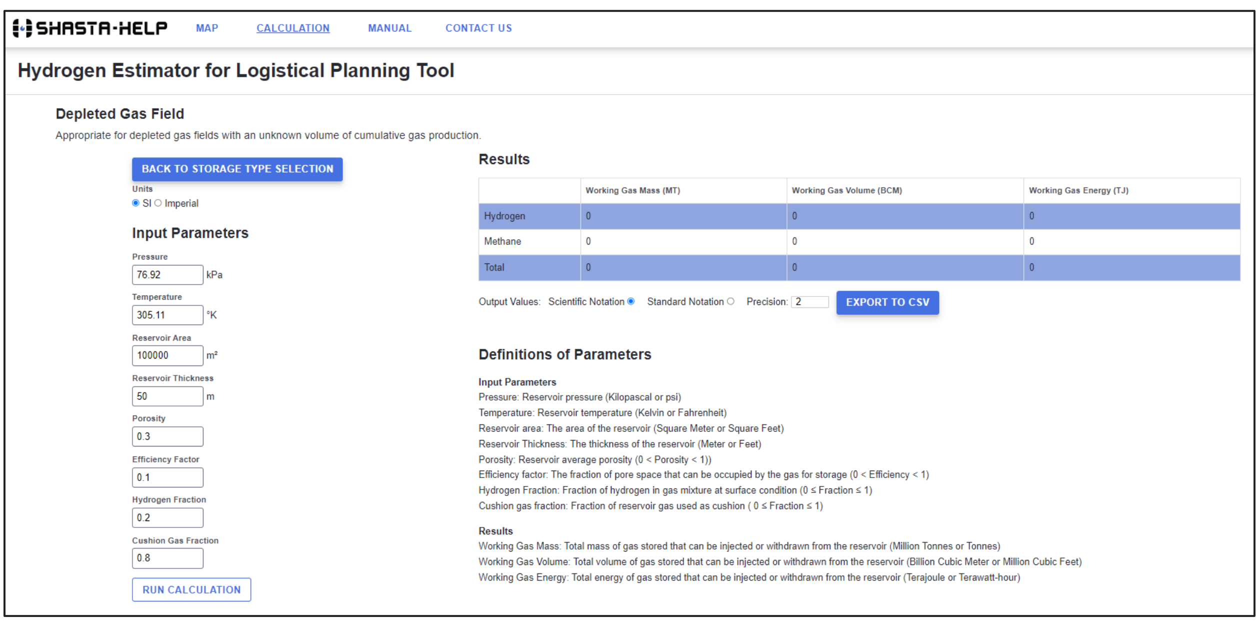

Figure 4.5: "Depleted Gas Field" page of SHASTA-HELP web-based tool when the cumulative gas production is unknown.

SALINE AQUIFER

If "Saline Aquifer" is selected from the "Prospective Geologic Formation" category on the main page (as shown in Figure 4.6), a new page will be displayed as shown in Figure 4.7 for calculations related to saline aquifers. The functionality of the unit radio button, input parameters, run button, and results table are as described before.

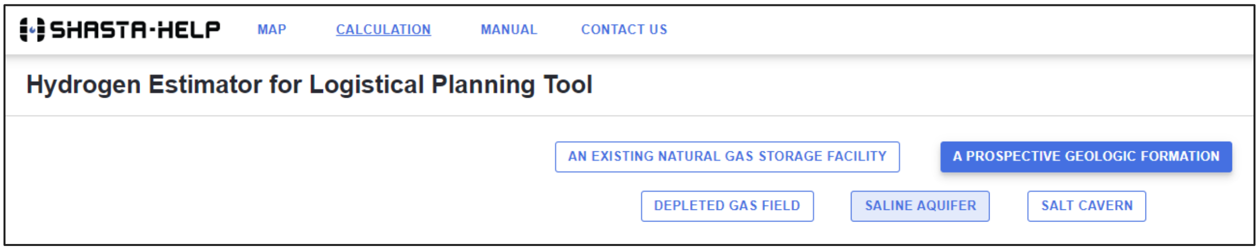

Figure 4.6: Selecting the "Saline Aquifer" option from "A Prospective Geologic Formation" category on the main page.

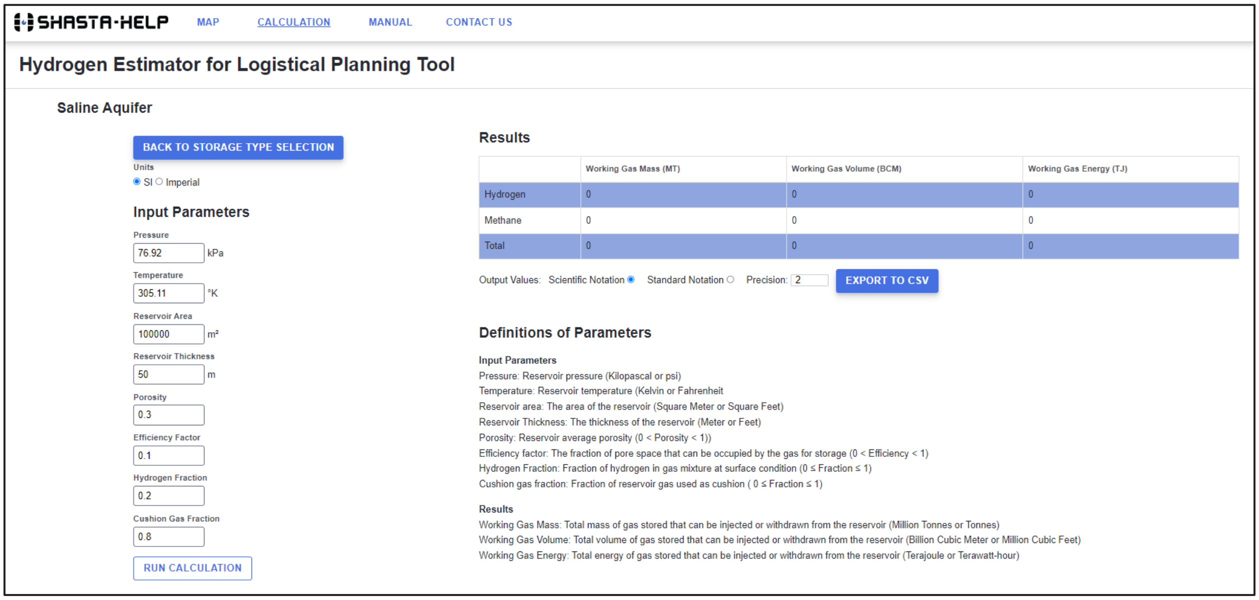

Figure 4.7: "Saline Aquifer" page of SHASTA-HELP web-based tool.

SALT CAVERN

If "Salt Cavern" is selected from the "Prospective Geologic Formation" category on the main page (as shown in Figure 4.8), a new page will be displayed for calculations related to salt caverns.

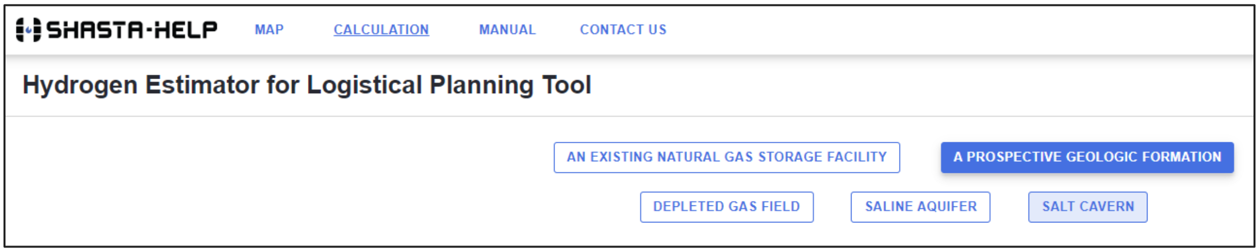

Figure 4.8: Selecting "Salt Cavern" option from "A Prospective Geologic Formation" category on the main page.

These calculations can be performed for either a "Single cavern with specified information" or "Multiple equally sized caverns in a formation." An additional radio button is provided under "Input Parameters" to switch between these two modes. Figure 4.9 shows the page for calculations related to a single cavern (default mode of the radio button) and Figure 4.10 shows the page for calculations related to multiple caverns. The functionality of the unit radio button, input parameters, run button, and results table are as described before.

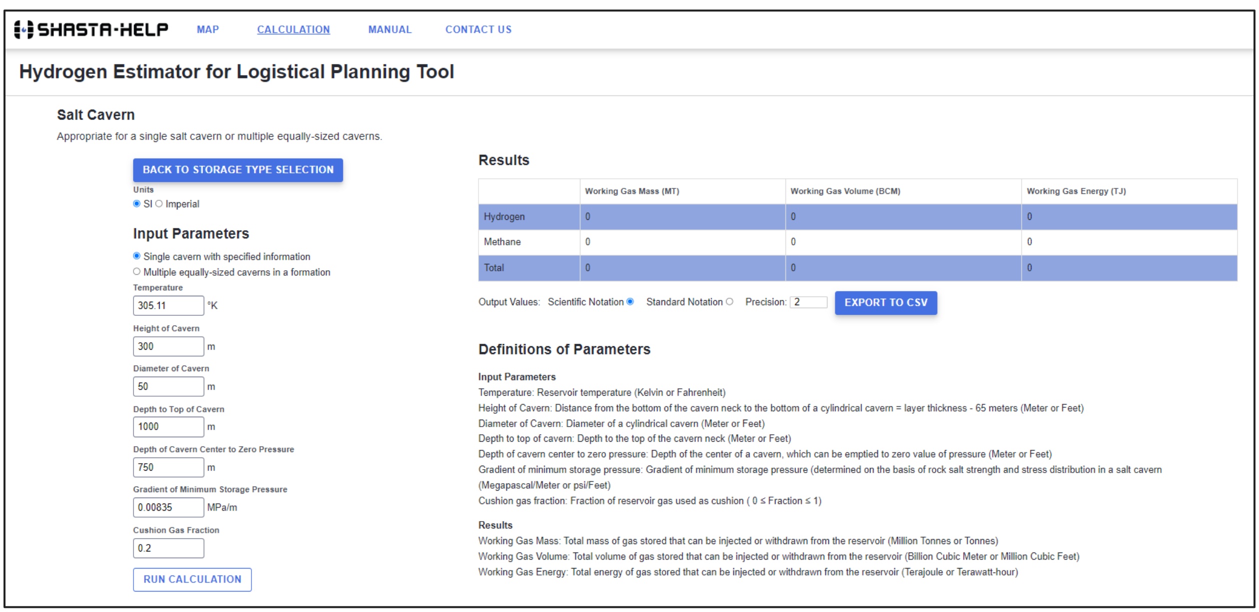

Figure 4.9: "Salt Cavern (single)" page of SHASTA-HELP web-based tool.

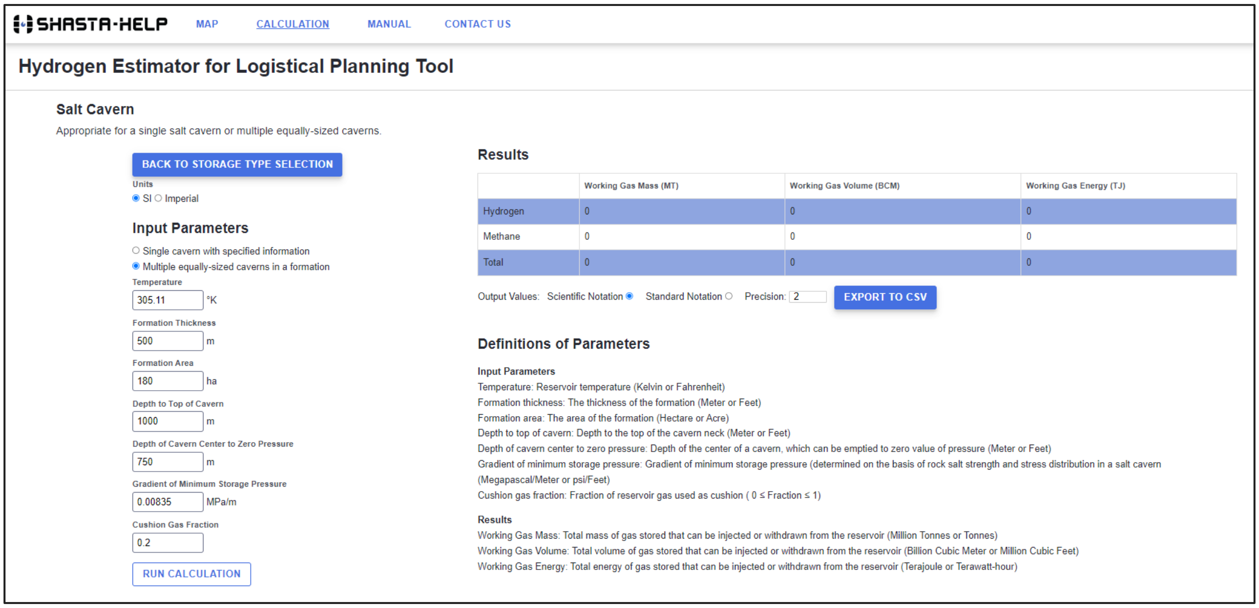

Figure 4.10: "Salt Cavern (multiple)" page of SHASTA-HELP web-based tool.

The step-by-step calculations used in the tool are provided in Appendices A–E for natural gas storage facilities, depleted gas fields, saline aquifers, and salt caverns. More details about the methodology can be found in Lackey et al. (2023).

5.0 References

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Appendix A: Calculation Steps for Natural Gas Storage Sites

Input parameters

Pressure: P_res

Temperature: T_res

Reported working gas volume: wgv_in

Hydrogen fraction: H2_frac_stp

Surface temperature and pressure

P_stp = 1 bar

T_stp = 273.15 K

Heating value of H_2 and CH_4

lhv_H2 = 3.332e-8 Twh/kg

lhv_CH4 = 1.389e-8 Twh/kg

Fraction of CH_4 in gas

CH4_frac_stp = 1 - H2_frac_stp

Density of H_2 and CH_4 at surface and reservoir conditions

rho_H2_stp: estimated at P_stp and T_stp using Peng-Robinson equation of state

rho_CH4_stp: estimated at P_stp and T_stp using Peng-Robinson equation of state

rho_H2_res: estimated at P_res and T_res using Peng-Robinson equation of state

rho_CH4_res: estimated at P_res and T_res using Peng-Robinson equation of state

H_2 and CH_4 fraction in gas at reservoir conditions

if H2_frac_stp = 1 then:

H2_frac_res = H2_frac_stp

CH4_frac_res = CH4_frac_stp

If H2_frac_stp ≠ 1 then:

H2_frac_res = ((rho_H2_stp / rho_H2_res) * H2_frac_stp) /

(((rho_H2_stp / rho_H2_res) * H2_frac_stp) + ((rho_CH4_stp / rho_CH4_res) * CH4_frac_stp))

CH4_frac_res = 1 - H2_frac_res

Calculate working gas mass (wgm) results

wgm_H2 = rho_H2_res * H2_frac_res * (rho_CH4_stp / rho_CH4_res) * wgv_in

wgm_CH4 = rho_CH4_res * CH4_frac_res * (rho_CH4_stp / rho_CH4_res) * wgv_in

wgm_total = wgm_H2 + wgm_CH4

Calculate working gas energy (wge) results

wge_H2 = lhv_H2 * rho_H2_res * H2_frac_res * (rho_CH4_stp / rho_CH4_res) * wgv_in

wge_CH4 = lhv_CH4 * rho_CH4_res * CH4_frac_res * (rho_CH4_stp / rho_CH4_res) * wgv_in

wge_total = wge_H2 + wge_CH4

Calculate working gas volume (wgv) results

wgv_H2 = (rho_H2_res / rho_H2_stp) * H2_frac_res * (rho_CH4_stp / rho_CH4_res) * wgv_in

wgv_CH4 = (rho_CH4_res / rho_CH4_stp) * CH4_frac_res * (rho_CH4_stp / rho_CH4_res) * wgv_in

wgv = wgv_H2 + wgv_CH4

Appendix B: Calculation Steps for Depleted Gas Fields

Input parameters

Pressure: P_res

Temperature: T_res

Cumulative produced gas: V_res

Hydrogen fraction: H2_frac_stp

Cushion gas fraction: cg_frac

Surface temperature and pressure

P_stp = 1 bar

T_stp = 273.15 K

Heating value of H_2 and CH_4

lhv_H2 = 3.332e-8 Twh/kg

lhv_CH4 = 1.389e-8 Twh/kg

Fraction of CH_4 in gas

CH4_frac_stp = 1 - H2_frac_stp

Density of H_2 and CH_4 at surface and reservoir conditions

rho_H2_stp: estimated at P_stp and T_stp using Peng-Robinson equation of state

rho_CH4_stp: estimated at P_stp and T_stp using Peng-Robinson equation of state

rho_H2_res: estimated at P_res and T_res using Peng-Robinson equation of state

rho_CH4_res: estimated at P_res and T_res using Peng-Robinson equation of state

H_2 and CH_4 fraction in gas at reservoir conditions

if H2_frac_stp = 1 then:

H2_frac_res = H2_frac_stp

CH4_frac_res = CH4_frac_stp

If H2_frac_stp ≠ 1 then:

H2_frac_res = ((rho_H2_stp / rho_H2_res) * H2_frac_stp) /

(((rho_H2_stp / rho_H2_res) * H2_frac_stp) + ((rho_CH4_stp / rho_CH4_res) * CH4_frac_stp))

CH4_frac_res = 1 - H2_frac_res

Calculate working gas mass (wgm) results

wgm_H2 = (rho_H2_res * H2_frac_res * (rho_CH4_stp / rho_CH4_res) * V_res*(1-cg_frac)

wgm_CH4 = (rho_CH4_res * CH4_frac_res * (rho_CH4_stp / rho_CH4_res) * V_res*(1-cg_frac)

wgm_total = wgm_H2 + wgm_CH4

Calculate working gas energy (wge) results

wge_H2 = lhv_H2 * rho_H2_res * H2_frac_res * (rho_CH4_stp / rho_CH4_res) * V_res*(1-cg_frac)

wge_CH4 = lhv_CH4 * rho_CH4_res * CH4_frac_res * (rho_CH4_stp / rho_CH4_res) * V_res*(1-cg_frac)

wge_total = wge_H2 + wge_CH4

Calculate working gas volume (wgv) results

wgv_H2 = (rho_H2_res / rho_H2_stp) * H2_frac_res * (rho_CH4_stp / rho_CH4_res) * V_res*(1-cg_frac)

wgv_CH4 = (rho_CH4_res / rho_CH4_stp) * CH4_frac_res * (rho_CH4_stp / rho_CH4_res) * V_res*(1-cg_frac)

wgv = wgv_H2 + wgv_CH4

Appendix C: Calculation Steps for Saline Aquifers

Input parameters

Pressure: P_res

Temperature: T_res

Reservoir area: A_res

Reservoir thickness: H_res

Porosity: phi_res

Efficiency factor: ef

Hydrogen fraction: H2_frac_stp

Cushion gas fraction: cg_frac

Surface temperature and pressure

P_stp = 1 bar

T_stp = 273.15 K

Heating value of H_2 and CH_4

lhv_H2 = 3.332e-8 Twh/kg

lhv_CH4 = 1.389e-8 Twh/kg

Fraction of CH_4 in gas

CH4_frac_stp = 1 - H2_frac_stp

Density of H_2 and CH_4 at surface and reservoir conditions

rho_H2_stp: estimated at P_stp and T_stp using Peng-Robinson equation of state

rho_CH4_stp: estimated at P_stp and T_stp using Peng-Robinson equation of state

rho_H2_res: estimated at P_res and T_res using Peng-Robinson equation of state

rho_CH4_res: estimated at P_res and T_res using Peng-Robinson equation of state

H_2 and CH_4 fraction in gas at reservoir conditions

if H2_frac_stp = 1 then:

H2_frac_res = H2_frac_stp

CH4_frac_res = CH4_frac_stp

If H2_frac_stp ≠ 1 then:

H2_frac_res = ((rho_H2_stp / rho_H2_res) * H2_frac_stp) /

(((rho_H2_stp / rho_H2_res) * H2_frac_stp) + ((rho_CH4_stp / rho_CH4_res) * CH4_frac_stp))

CH4_frac_res = 1 - H2_frac_res

Calculate working gas mass (wgm) results

wgm_H2 = (rho_H2_res * H2_frac_res * (rho_CH4_stp / rho_CH4_res) * A_res*H_res*phi_res*ef*(1-cg_frac)

wgm_CH4 = (rho_CH4_res * CH4_frac_res * (rho_CH4_stp / rho_CH4_res) * A_res*H_res*phi_res*ef*(1-cg_frac)

wgm_total = wgm_H2 + wgm_CH4

Calculate working gas energy (wge) results

wge_H2 = lhv_H2 * rho_H2_res * H2_frac_res * (rho_CH4_stp / rho_CH4_res) * A_res*H_res*phi_res*ef*(1-cg_frac)

wge_CH4 = lhv_CH4 * rho_CH4_res * CH4_frac_res * (rho_CH4_stp / rho_CH4_res) * A_res*H_res*phi_res*ef*(1-cg_frac)

Calculate working gas volume (wgv) results

wgv_H2 = (rho_H2_res / rho_H2_stp) * H2_frac_res * (rho_CH4_stp / rho_CH4_res) * A_res*H_res*phi_res*ef*(1-cg_frac)

wgv_CH4 = (rho_CH4_res / rho_CH4_stp) * CH4_frac_res * (rho_CH4_stp / rho_CH4_res) * A_res*H_res*phi_res*ef*(1-cg_frac)

wgv = wgv_H2 + wgv_CH4

Appendix D: Calculation Steps for Salt Caverns (Single Cavern, Pure Hydrogen)

Input parameters

Temperature: T_res

Height of cavern: H_cav

Diameter of cavern: D_cav

Depth to top of cavern: h_n

Depth of cavern center to zero pressure: h_o

Gradient of minimum storage pressure: g_min

Cushion gas fraction: cg_frac

Fracture gradient

g_f = 0.016 Mpa/m

H_2 gas constant and density

R_h2 = 4121.73 KJ/kg K (universal gas constant/H2 molar mass)

rho_h2_n = 0.089 kg/m3 (at surface conditions: could be entered by user)

Depth to center of cavern

h_c = h_n + 15 + H_cav/2

Volume of cavern

V_cav = (π/ 12) * (D_cav^2)*(3 * H_cav - D_cav)

Maximum pressure

P_max = g_f * h_n

Minimum pressure

P_min = g_min * (h_c - h_o)

Maximum and minimum compressibility factors

Z_max: estimated at P_max and T_res using Peng-Robinson equation of state

Z_min: estimated at P_min and T_res using Peng-Robinson equation of state

Maximum and minimum mass stored

M_max = (1 - cg_frac) * ((P_max * V_cav) / R_h2 * T_res * Z_max)

M_min = (1 - cg_frac) * ((P_min * V_cav) / R_h2 * T_res * Z_min)

Working gas mass

wgm = M_max - M_min

Working gas energy

wge = wgm * lhv_H2

Working gas volume

wgv = (wgm / rho_h2_n)

Appendix E: Calculation Steps for Salt Caverns (Multiple Caverns, Pure Hydrogen)

Input parameters

Temperature: T_res

Formation thickness: F_thick (must be greater than 65 m)

Formation area: F_area (must be greater than $16*[2*(F\_thick – 65)/3]^2$)

Depth to top of cavern: h_n

Depth of cavern center to zero pressure: h_o

Gradient of minimum storage pressure: g_min

Cushion gas fraction: cg_frac

Fracture gradient

g_f = 0.016 Mpa/m

H_2 gas constant and density

R_h2 = 4121.73 KJ/kg K (universal gas constant/H2 molar mass)

rho_h2_n = 0.089 kg/m3 (at surface conditions: could be entered by user)

Cavern density in space

cav_den = 0.0000185 caverns/m**2 (1 cavern/5.4 hectare) - Lankof and Tarkowski (2020)

Depth to center of cavern

h_c = h_n + 15 + H_cav/2

Volume of cavern

$V\_cav = (\pi/ 12) * (D\_cav^2)*(3 * H\_cav - D\_cav)$

Maximum pressure

P_max = g_f * h_n

Minimum pressure

P_min = g_min * (h_c - h_o)

Maximum and minimum compressibility factors

Z_max: estimated at P_max and T_res using Peng-Robinson equation of state

Z_min: estimated at P_min and T_res using Peng-Robinson equation of state

Maximum and minimum mass stored

M_max = (1 - cg_frac) * ((P_max * V_cav) / R_h2 * T_res * Z_max)

M_min = (1 - cg_frac) * ((P_min * V_cav) / R_h2 * T_res * Z_min)

Working gas mass per cavern

wgm_pc = M_max - M_min

Working gas energy

wge = wgm_pc * lhv_H2

Working gas volume

wgv = (wgm_pc / rho_h2_n)* 0.00003531 (m3 to MMcf)

Number of caverns in formation

n_cav = F_area*cav_den

Total mass, energy, and for formation

wgm = wgm_pc * n_cav

wge = wge_pc * n_cav

wgv = wgv_pc * n_cav

Appendix F: Definitions of Parameters Used to Calculate the Working Gas Energy of H_2 Storage

Table F.1: Description of Parameters used in Equations (1) to (6).

Parameter	Unit	Description
WGE_{H_2}	TWh	Working gas energy of H_2 at the ground surface conditions at 101.56 kPa and 15.56 ˚C
WGE_{mix}	TWh	Working gas energy of blended H_2-CH_4 mixtures at the ground surface conditions at 101.56 kPa and 15.56 ˚C
LHV_{H_2}	$\frac{kWh}{kg}$	Lower heating value of H_2 (120 MJ/kg)
LHV_{CH_4}	$\frac{kWh}{kg}$	Lower heating value of CH_4 (50 MJ/kg)
$\rho_{H_2,r}$	$\frac{kg}{m^3}$	Density of H_2 in the storage reservoir at storage conditions when the reservoir is full
$\rho_{H_2,a}$	$\frac{kg}{m^3}$	Density of H_2 at the ground surface conditions (101.56 kPa and 15.56 ˚C)
$\rho_{H_2,STP}$	$\frac{kg}{m^3}$	Density of H_2 at standard temperature and pressure (STP) at 100 kPa and 0 ˚C
$\rho_{CH_4,r}$	$\frac{kg}{m^3}$	Density of CH_4 in the storage reservoir at storage conditions when the reservoir is full
$\rho_{CH_4,a}$	$\frac{kg}{m^3}$	Density of CH_4 at the ground surface conditions (101.56 kPa and 15.56 ˚C)
$\rho_{CH_4,STP}$	$\frac{kg}{m^3}$	Density of CH_4 at standard temperature and pressure (STP) at 100 kPa and 0 ˚C
$VF_{H_2,r}$	*fraction*	Volume fraction of H_2 in the mixture at storage conditions when the reservoir is full
$VF_{CH_4,r}$	*fraction*	Volume fraction of CH_4 in the mixture at storage conditions when the reservoir is full
$VF_{H_2,STP}$	*fraction*	Volume fraction of H_2 in the mixture at standard temperature and pressure (STP) at 100 kPa and 0 ˚C
$VF_{CH_4,STP}$	*fraction*	Volume fraction of CH_4 in the mixture at standard temperature and pressure (STP) at 100 kPa and 0 ˚C
$WGV_{H_{2,a}}$	m^3	Working gas volume of H_2 at the ground surface conditions at 101.56 kPa and 15.56 ˚C
$WGV_{CH_{4,a}}$	m^3	Working gas volume of CH_4 at the ground surface conditions in the EIA dataset at 101.56 kPa and 15.56 ˚C
$WGV_{H_2,mix}$	m^3	Working gas volume of blended H_2 at the ground surface conditions at 101.56 kPa and 15.56 ˚C
$WGV_{CH_4,mix}$	m^3	Working gas volume of blended CH_4 at the ground surface conditions in the EIA dataset at 101.56 kPa and 15.56 ˚C

Appendix G: Running The Downloadable Version of the SHASTA-HELP Tool

The downloadable version of the SHASTA-HELP tool is publicly available on GitHub and can be found here: https://github.com/netl-ric/wgv_calculation. This version is coded in the Python computer programming language. The tool can be imported as a Python module or interacted with through the built-in Graphical User Interface (GUI).

Figure G.1 shows the screenshot of the GitHub repository. The Python libraries required to run the tool are as follow:

- python = 3.7.6
- numpy = 1.20.3
- scipy = 1.7.3
- PIL = 7.0.0
- tkinter = 8.6.8

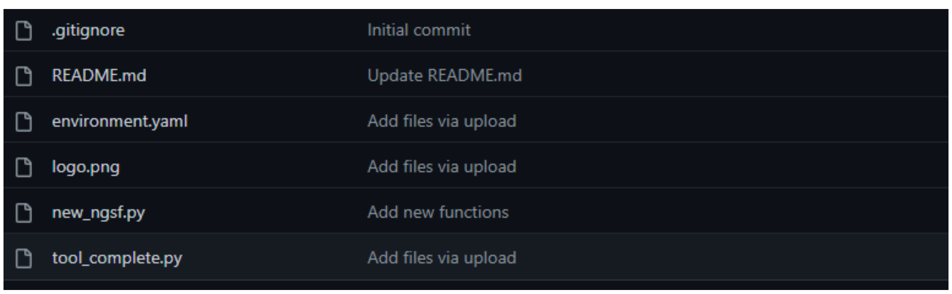

Figure G.1: Screenshot of the downloadable version of SHASTA-HELP tool on GitHub.

GETTING STARTED

To use the downloadable version, after running the file "tool_complete.py," the GUI splash page will appear as shown in Figure G.2. The first step is to select a formation by clicking on "Select a formation" and choosing the target formation from the dropdown.

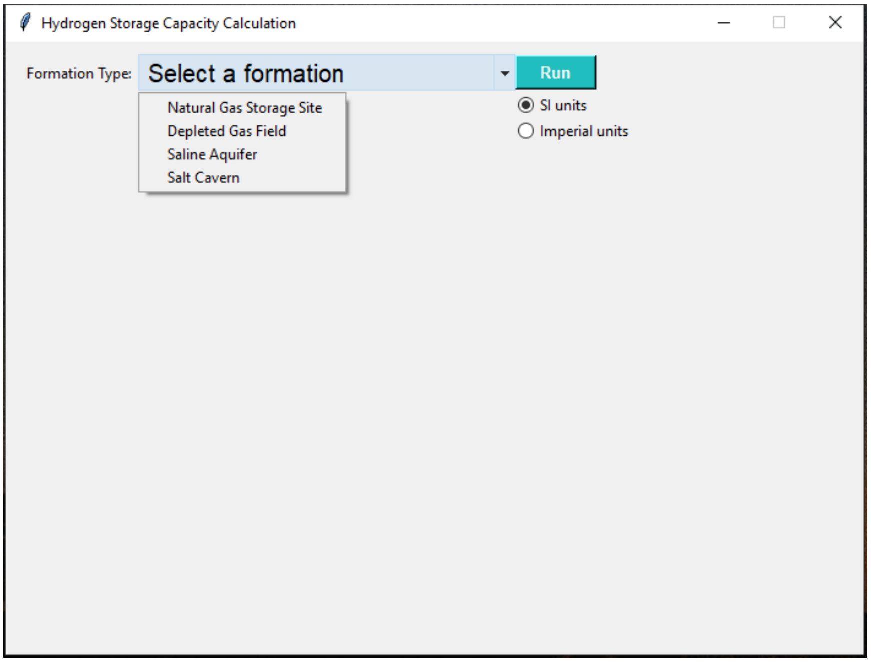

Figure G.2: Screenshot of the SHASTA-HELP tool GUI splash page, including a dropdown to select formation.

INPUT PARAMETERS

The dropdown for target formation has four options, including:

- Natural Gas Storage Site
- Depleted Gas Field
- Saline Aquifer
- Salt Cavern

By selecting any of the options in the dropdown, a list of input parameters and their respective default values will appear as shown in Figures G.3–G.7. To switch the unit, use the radio button under the green "Run" button at the top of the window. Every time you change the unit, a prompt message will appear notifying you that the unit is changing, and you will have to start over by selecting the formation again. When you select a formation, input parameters will have default values with the new selected unit. The default values are provided to give some hints to the user. Values can always be modified to new values entered by the user. Note that for salt cavern calculations only pure hydrogen is considered in this version of the tool. When salt cavern is selected as the target formation, a radio button appears to provide the choice between "Single cavern with specified information" (Figure G.6) or "Multiple equally-sized caverns in a formation" (Figure G.7), for each of which specific input parameters will be listed.

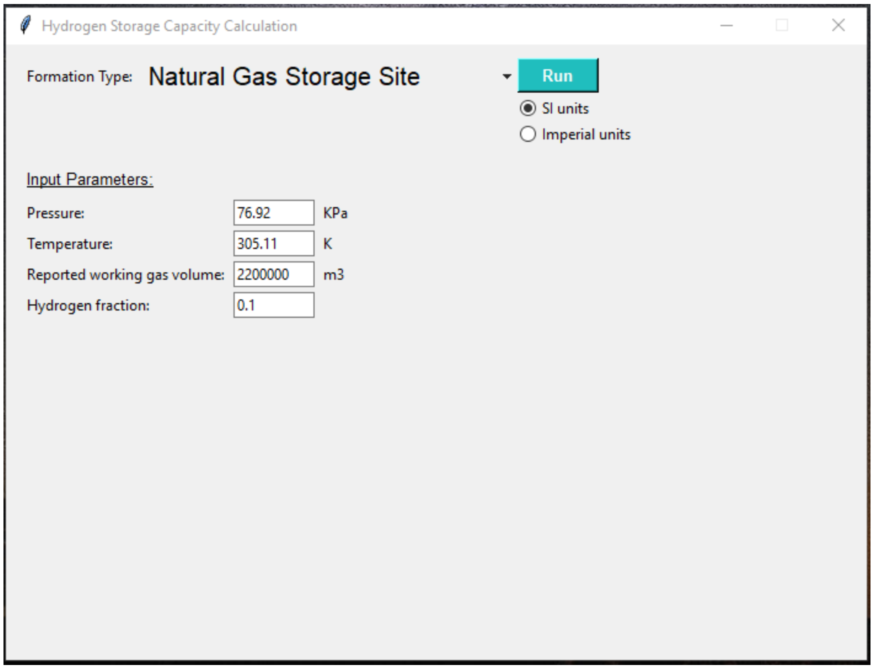

Figure G.3: Screenshot of the SHASTA-HELP tool GUI – Input Parameters for Natural Gas Storage Site.

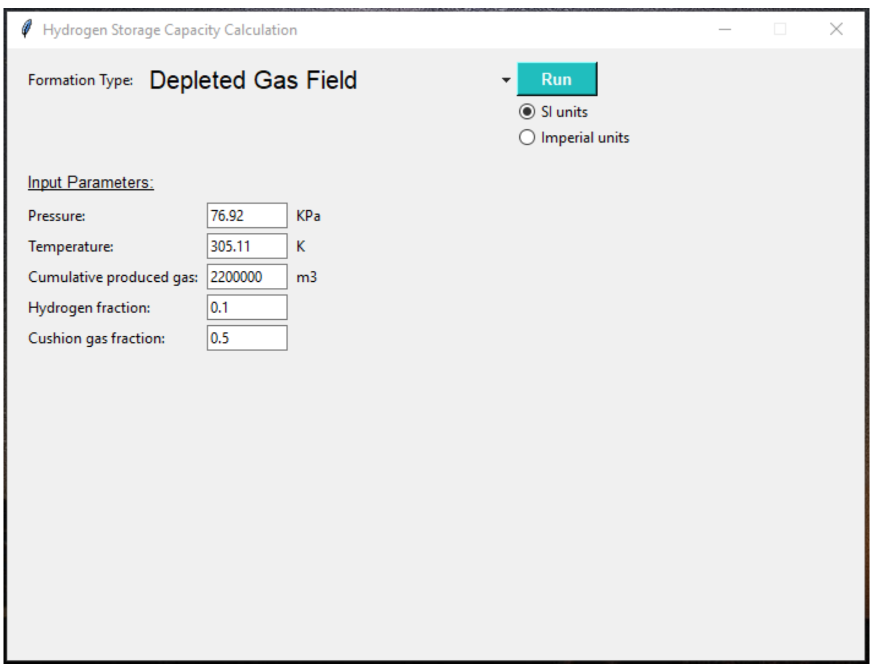

Figure G.4: Screenshot of the SHASTA-HELP tool GUI – Input Parameters for Depleted Gas Field.

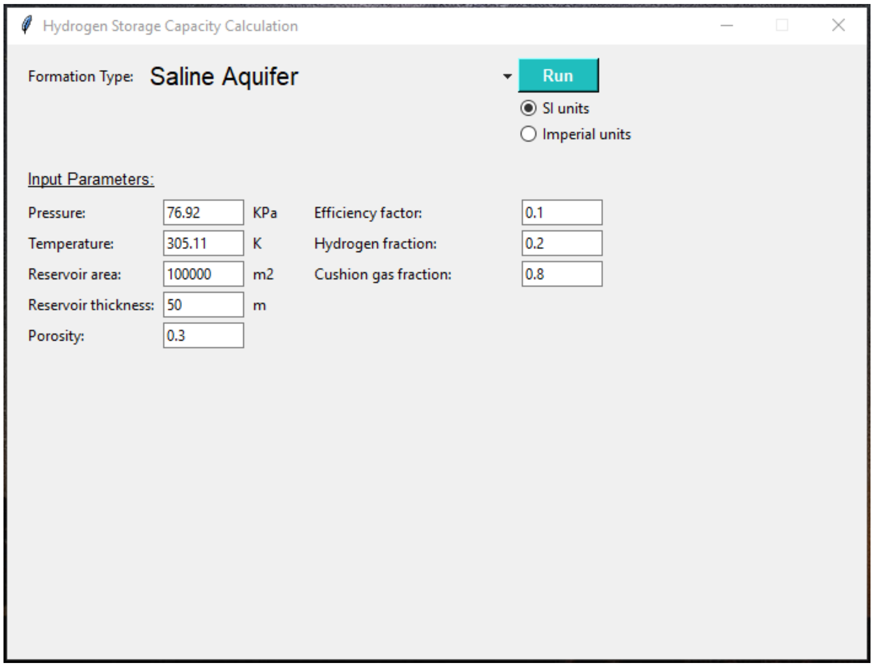

Figure G.5: Screenshot of the SHASTA-HELP tool GUI – Input Parameters for Saline Aquifer.

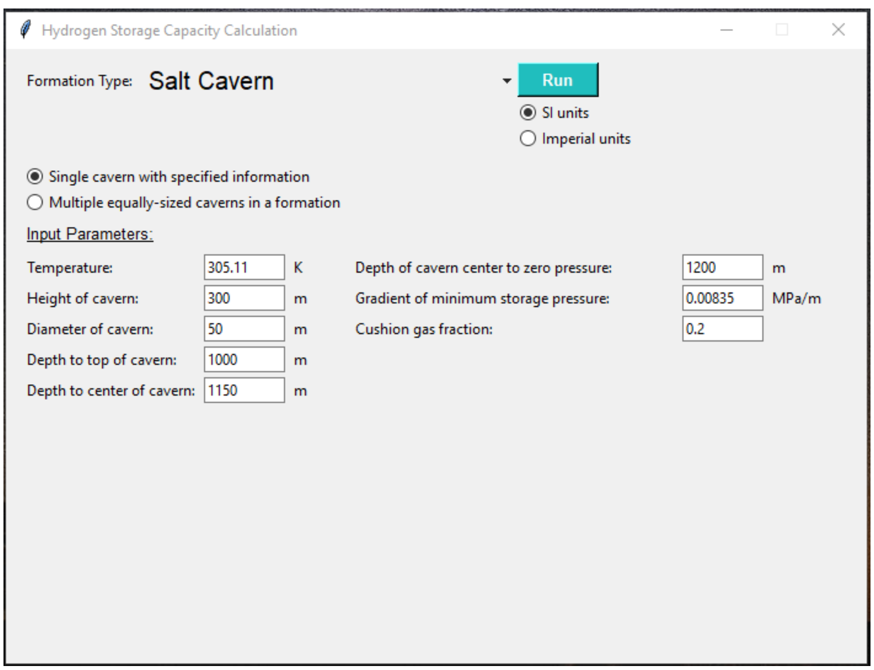

Figure G.6: Screenshot of the SHASTA-HELP tool GUI – Input Parameters for Salt Cavern (single).

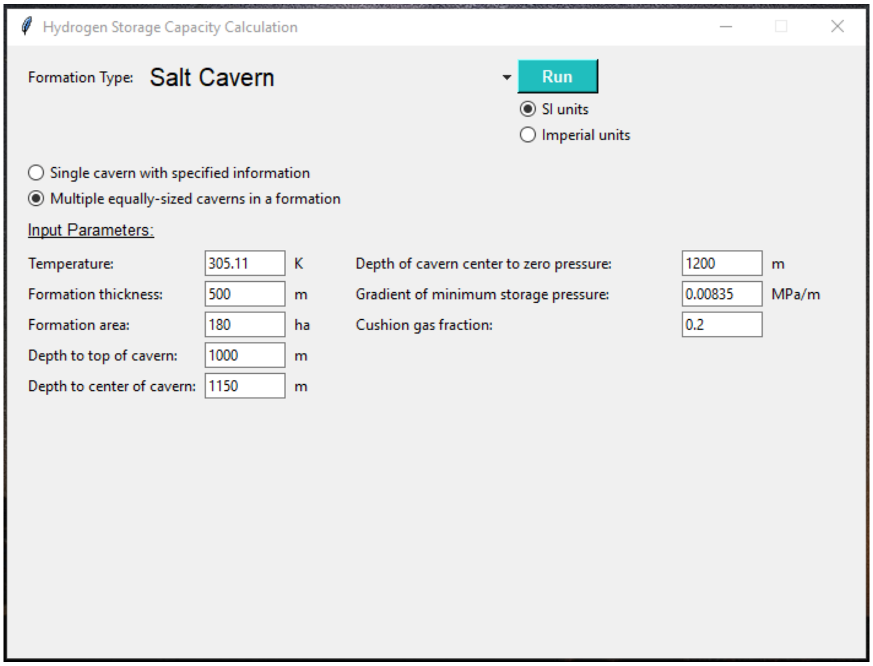

Figure G.7: Screenshot of the SHASTA-HELP tool GUI – Input Parameters for Salt Cavern (multiple).

RESULTS

Once input parameters are finalized with default or modified values (all entries must contain a value), press the green "Run" button at the top of the window (Figure G.8). When the calculations are completed, the results will appear at the bottom of the window. The results include the working gas mass, working gas volume, and working gas energy of hydrogen, methane, and total blend.

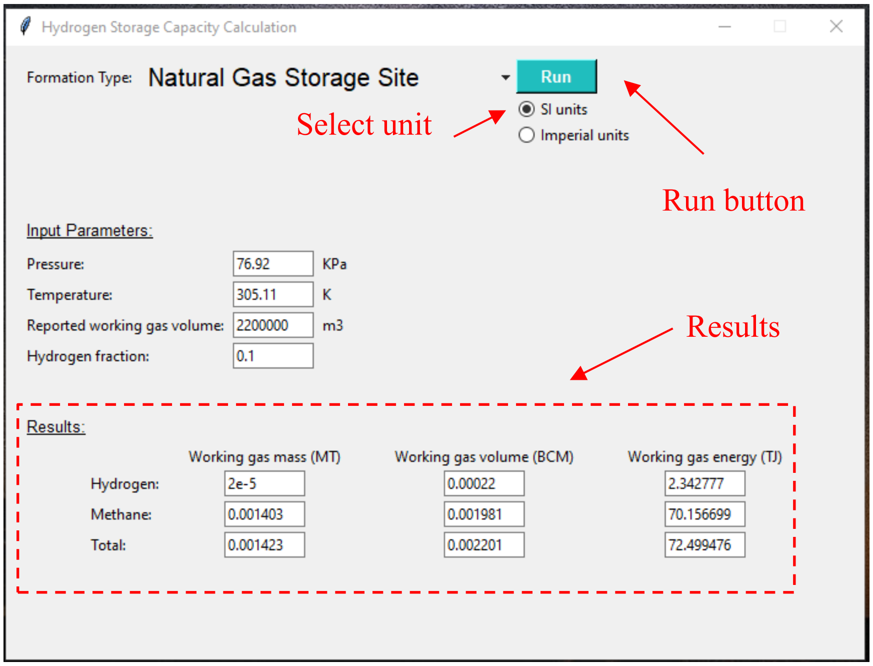

Figure G.8: Screenshot of the SHASTA-HELP tool GUI – The Unit, "Run" button, and Results.

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