

INTEGRATED MODEL FOR DETERMINING THE RESERVOIR ROCK PROPERTIES DURING UNDERGROUND STORAGE OF A GAS-HYDROGEN MIXTURE

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Abstract. An integrated model for determining the reservoir properties of the rock reservoir during underground storage of a gas-hydrogen mixture is presented. The methodology consists of four main modules: Characterization of the core sample (mineral composition, porosity, and permeability), determination of the parameters of the gas-hydrogen mixture at different % hydrogen and methane contents (5%, 15%, 25%), study of flow properties (porosity and permeability of the core sample at different gas-hydrogen mixture contents), and a module summarizing the results. The results obtained from the study using the developed methodology form the basis for designing the storage indicators for gas-hydrogen mixtures in underground gas storage facilities.

Keywords: hydrogen; underground storage; capacitance parameters; flow parameters

Introduction

The main objective of the paper is to investigate and study the effect of hydrogen on the capacity and flow parameters of the rock, as hydrogen has emerged as a promising alternative to address the growing demand for sustainable and renewable energy sources. Underground hydrogen storage (UHS) in depleted gas fields has significant potential for large-scale energy storage and seamless integration of renewable energy sources due to its ability to address the challenges associated with the intermittent nature of renewable energy sources, ensuring a stable and reliable energy supply (Gerov, 2019). Due to the impact of exhaust gases on nature, action is needed to decarbonize the atmosphere. This can be done through the use of hydrogen gas mixtures for domestic and industrial use. In the following publication, the influence of gas- hydrogen mixtures on the hydro-gas-dynamic parameters of reservoir rocks in a gas field and in particular on the near-hole zone where the wellbore-productive horizon contact takes place is investigated.

An integrated model for determining the reservoir properties of the rock reservoir during underground storage of a gas-hydrogen mixture is presented on

Figure 1. It consists of four main modules: Characterization of the core sample (mineral composition, porosity, and permeability), determination of the parameters of the gas-hydrogen mixture at different % hydrogen and methane contents (5%, 15%, 25%), study of flow properties (porosity and permeability of the core sample at different gas-hydrogen mixture contents), and a module summarizing the results. The porosity of the core sample is determined using two methods: tomography and a helium porosimeter. When using the tomography method, the mineralogical and petrographic composition of the core (extracted from the rock reservoir) is also determined (Lakov et al., 2024).

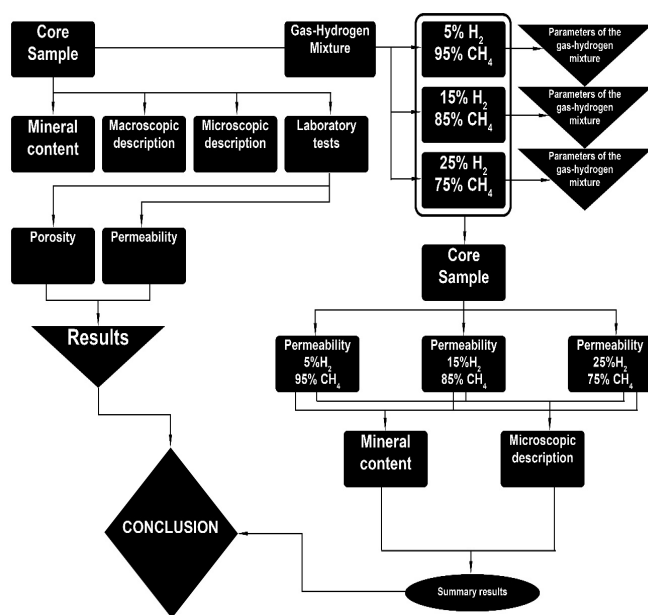


Figure 1. Block scheme of the integrated model

Based on the presented integrated model, the parameters of the gas-hydrogen mixture are determined, as presented below.

Experimental

Each gas mixture consists of a set of components, and each individual component has its own parameters: molar mass, critical pressure, critical temperature, relative density, etc. The corresponding gas mixture has the same parameters. Table 1 shows an example of a hydrogen gas mixture.

Table 1. Certificate of the gas-hydrogen mixture

Gas mixture certificate						
	Component	Percentage content	Molar mass of the component	Critical pressure	Critical temperature	Relative density
Unit of measurement		mol %	kg.kmol ⁻¹	MPa	K	
5% H ₂	Methane CH ₄	95.00	16.043	4.605	190.6	0.5539
	Hydrogen H ₂	5.00	2.016	1.299	33.3	0.0696
	Total:	100.00				
15% H ₂	Methane CH ₄	85.00	16.043	4.605	190.6	0.5539
	Hydrogen H ₂	15.00	2.016	1.299	33.3	0.0696
	Total:	100.00				
25% H ₂	Methane CH ₄	75.00	16.043	4.605	190.6	0.5539
	Hydrogen H ₂	25.00	2.016	1.299	33.3	0.0696
	Total:	100.00				

Relative density, also called specific gravity, is a dimensionless quantity defined as the ratio of the density (*mass divided by volume*) of a substance to the density of a given reference material or substance. The term “relative density” (abbreviated r.d. or RD) is preferred in SI, whereas the term “specific gravity” is gradually being abandoned. The relative density of gases is often measured with respect to dry air at a temperature of 20 °C and a pressure of 101.325 kPa absolute, which has a density of 1.205 kg.m⁻³. Relative density with respect to air can be obtained by formula 1.

$$RD = \frac{\rho_{gas}}{\rho_{air}} \quad (1)$$

Where:

ρ_{gas} – density of the measured gas [kg.m⁻³]

ρ_{air} – density of air [kg.m⁻³]

Using formula 2, we calculate the molecular mass of the gas-hydrogen mixture; the data is taken from the gas-hydrogen mixture certificate (Boyadjiev & Georgiev, 2020; Nikolov, 1993).

$$M_{gm} = \frac{\sum_{i=1}^n M_i \times x_i}{100}, [kg.kmol^{-1}] \quad (2)$$

Where:

M_i – molar mass of component i in the gas-hydrogen mixture [kg.kmol⁻¹]

X_i – percentage content of component i in the gas-hydrogen mixture [mol %]

Table 2. Calculation of the molecular mass of the gas-hydrogen mixture

% H ₂ content	Molecular mass of the gas-hydrogen mixture	xi . Mi	kg.kmol ⁻¹
5 % H ₂	Methane CH ₄	15.2409	kg.kmol ⁻¹
	Hydrogen H ₂	0.1008	kg.kmol ⁻¹
	Molecular mass of the gas-hydrogen mixture	15.3417	kg.kmol ⁻¹
15 % H ₂	Methane CH ₄	13.6366	kg.kmol ⁻¹
	Hydrogen H ₂	0.3024	kg.kmol ⁻¹
	Molecular mass of the gas-hydrogen mixture	13.9390	kg.kmol ⁻¹
25 % H ₂	Methane CH ₄	12.0323	kg.kmol ⁻¹
	Hydrogen H ₂	0.5040	kg.kmol ⁻¹
	Molecular mass of the gas-hydrogen mixture	12.5363	kg.kmol ⁻¹

Using formula 3, we calculate the critical pressure of the gas-hydrogen mixture; the data is taken from the gas-hydrogen mixture certificate.

$$P_{crit} = \frac{\sum_{i=1}^n P_{criti} \times x_i}{100} \quad (3)$$

Where:

P_{criti} – critical pressure of the i component in the gas-hydrogen mixture [MPa]

X_i – percentage content of component i in the gas-hydrogen mixture [mol %]

Table 3. Critical pressure of the gas-hydrogen mixture

% H ₂ content	Critical pressure of the gas-hydrogen mixture	xi . Pkri	MPa
5 % H ₂	Methane CH ₄	4.3748	MPa
	Hydrogen H ₂	0.0650	MPa
	Critical pressure of the gas-hydrogen mixture	4.4397	MPa
15 % H ₂	Methane CH ₄	3.9143	MPa
	Hydrogen H ₂	0.1949	MPa
	Critical pressure of the gas-hydrogen mixture	4.1091	MPa

25 % H ₂	Methane CH ₄	3.4538	MPa
	Hydrogen H ₂	0.3248	MPa
	Critical pressure of the gas-hydrogen mixture	3.7785	MPa

Using formula 4, we calculate the critical temperature of the gas-hydrogen mixture; the data is taken from the gas-hydrogen mixture certificate.

$$T_{crit} = \frac{\sum_{i=1}^n T_{criti} \times x_i}{100} \quad (4)$$

Where:

T_{criti} – critical temperature of the i component in the gas-hydrogen mixture [K]

X_i – percentage content of component i in the gas-hydrogen mixture [mol %]

Table 4. Critical temperature of the gas-hydrogen mixture

% H ₂ content	Critical temperature of the gas-hydrogen mixture	xi . Tcriti	K
5 % H ₂	Methane CH ₄	181.070	K
	Hydrogen H ₂	1.665	K
	Critical temperature of the gas-hydrogen mixture	182.735	K
15 % H ₂	Methane CH ₄	162.010	K
	Hydrogen H ₂	4.995	K
	Critical temperature of the gas-hydrogen mixture	167.005	K
25 % H ₂	Methane CH ₄	142.950	K
	Hydrogen H ₂	8.325	K
	Critical temperature of the gas-hydrogen mixture	151.275	K

Formula 5 is used to calculate the density of the gas-hydrogen mixture under standard conditions (Temperature = 293.15 K; Pressure = 0.1013 MPa).

$$\rho_{gmst} = \frac{\left(\frac{\sum_{i=1}^n M_i \times x_i}{100} \right)}{24.04} \quad (5)$$

Table 5. Gas density under standard conditions

% H ₂ content	Density of the gas mixture under standard conditions (293.15 K; 0.1013 MPa)	[(xi.mi)/100]/24.04	kg.m ⁻³
5 % H ₂	Density of the gas mixture	0.6382	kg.m ⁻³
15 % H ₂	Density of the gas mixture	0.5798	kg.m ⁻³
25 % H ₂	Density of the gas mixture	0.5215	kg.m ⁻³

Formula 6 is used to calculate the relative density of the gas-hydrogen mixture.

$$\bar{\rho} = \frac{\rho_{gmst}}{1.2045} \quad (6)$$

Where:

ρ_{gmst} – density of the gas-hydrogen mixture at standard conditions [kg.m⁻³]

1.2045 – density of air at standard conditions [kg.m⁻³]

Table 6. Relative density of the gas-hydrogen mixture

% H ₂ content	Relative density of the gas mixture		
5 % H ₂	Density of air under standard conditions	1.2045	kg.m ⁻³
	Density of the gas mixture under standard conditions	0.6382	kg.m ⁻³
	Relative density of the gas mixture	0.530	
15 % H ₂	Density of air under standard conditions	1.2045	kg.m ⁻³
	Density of the gas mixture under standard conditions	0.5798	kg.m ⁻³
	Relative density of the gas mixture	0.481	
25 % H ₂	Density of air under standard conditions	1.2045	kg.m ⁻³
	Density of the gas mixture under standard conditions	0.5215	kg.m ⁻³
	Relative density of the gas mixture	0.433	

Formula 7 is used to calculate the derived pressure of the gas-hydrogen mixture.

$$P_{der} = \frac{P}{P_{crit}} \quad (7)$$

Where:

P – Pressure in the reservoir [MPa]

P_{crit} – Critical pressure of the gas-hydrogen mixture [MPa]

Table 7. Change in the derived pressure of the gas-hydrogen mixture with a change in the reservoir pressure

5 % H ₂	Critical pressure	4.4397	MPa	Derived pressure of the gas mixture	P _{der}
	Pressure 1	0.1	MPa	Derived pressure 1	0.0225
	Pressure 2	0.5	MPa	Derived pressure 2	0.1126
	Pressure 3	1	MPa	Derived pressure 3	0.2252
	Pressure 4	1.5	MPa	Derived pressure 4	0.3379
	Pressure 5	2	MPa	Derived pressure 5	0.4505
	Pressure 6	5	MPa	Derived pressure 6	1.1262
	Pressure 7	10	MPa	Derived pressure 7	2.2524
	Pressure 8	15	MPa	Derived pressure 8	3.3786
15 % H ₂	Critical pressure	4.1091	MPa	Derived pressure of the gas mixture	P _{der}
	Pressure 1	0.1	MPa	Derived pressure 1	0.0243
	Pressure 2	0.5	MPa	Derived pressure 2	0.1217
	Pressure 3	1	MPa	Derived pressure 3	0.2434
	Pressure 4	1.5	MPa	Derived pressure 4	0.3650
	Pressure 5	2	MPa	Derived pressure 5	0.4867
	Pressure 6	5	MPa	Derived pressure 6	1.2168
	Pressure 7	10	MPa	Derived pressure 7	2.4336
	Pressure 8	15	MPa	Derived pressure 8	3.6504
25 % H ₂	Critical pressure	3.7785	MPa	Derived pressure of the gas mixture	P _{der}
	Pressure 1	0.1	MPa	Derived pressure 1	0.0265
	Pressure 2	0.5	MPa	Derived pressure 2	0.1323
	Pressure 3	1	MPa	Derived pressure 3	0.2647
	Pressure 4	1.5	MPa	Derived pressure 4	0.3970
	Pressure 5	2	MPa	Derived pressure 5	0.5293
	Pressure 6	5	MPa	Derived pressure 6	1.3233
	Pressure 7	10	MPa	Derived pressure 7	2.6466
	Pressure 8	15	MPa	Derived pressure 8	3.9698

Formula 8 is used to calculate the derived pressure of the gas-hydrogen mixture.

$$T_{der} = \frac{T}{T_{crit}} \quad (8)$$

Where:

T – Temperature in the reservoir [K]

T_{crit} – Critical temperature of the gas-hydrogen mixture [K]

Table 8. Change in the derived temperature of the gas-hydrogen mixture with a change in the reservoir temperature

5 % H ₂	Critical temperature	182.73	K	Derived temperature of the gas mixture	T _{der}
	Temperature 1	273.15	K	Derived temperature 1	1.4948
	Temperature 2	278.15	K	Derived temperature 2	1.5221
	Temperature 3	283.15	K	Derived temperature 3	1.5495
	Temperature 4	288.15	K	Derived temperature 4	1.5769
	Temperature 5	293.15	K	Derived temperature 5	1.6042
	Temperature 6	298.15	K	Derived temperature 6	1.6316
	Temperature 7	303.15	K	Derived temperature 7	1.6590
	Temperature 8	308.15	K	Derived temperature 8	1.6863
15 % H ₂	Critical temperature	167.01	K	Derived temperature of the gas mixture	T _{der}
	Temperature 1	273.15	K	Derived temperature 1	1.6356
	Temperature 2	278.15	K	Derived temperature 2	1.6655
	Temperature 3	283.15	K	Derived temperature 3	1.6955
	Temperature 4	288.15	K	Derived temperature 4	1.7254
	Temperature 5	293.15	K	Derived temperature 5	1.7553
	Temperature 6	298.15	K	Derived temperature 6	1.7853
	Temperature 7	303.15	K	Derived temperature 7	1.8152
	Temperature 8	308.15	K	Derived temperature 8	1.8452
25 % H ₂	Critical temperature	151.27	K	Derived temperature of the gas mixture	T _{der}
	Temperature 1	273.15	K	Derived temperature 1	1.8057
	Temperature 2	278.15	K	Derived temperature 2	1.8387
	Temperature 3	283.15	K	Derived temperature 3	1.8718
	Temperature 4	288.15	K	Derived temperature 4	1.9048
	Temperature 5	293.15	K	Derived temperature 5	1.9379
	Temperature 6	298.15	K	Derived temperature 6	1.9709
	Temperature 7	303.15	K	Derived temperature 7	2.0040
	Temperature 8	308.15	K	Derived temperature 8	2.0370

Once we have found the derived pressure of a gas-hydrogen mixture with 5, 15, 25% H₂ content and, accordingly, the derived temperature of the same gas-hydrogen

mixture, but we have chosen only two temperatures – 288.15 K, 293.15 K, we can find the supercompressibility coefficient of the gas-hydrogen mixture at different pressures and two temperatures. The data is shown in Table 9,10,11 and is depicted in Graph 1, 2, 3. For this purpose, we have used the nomogram of “Standing and Katz” shown on Figure 2.

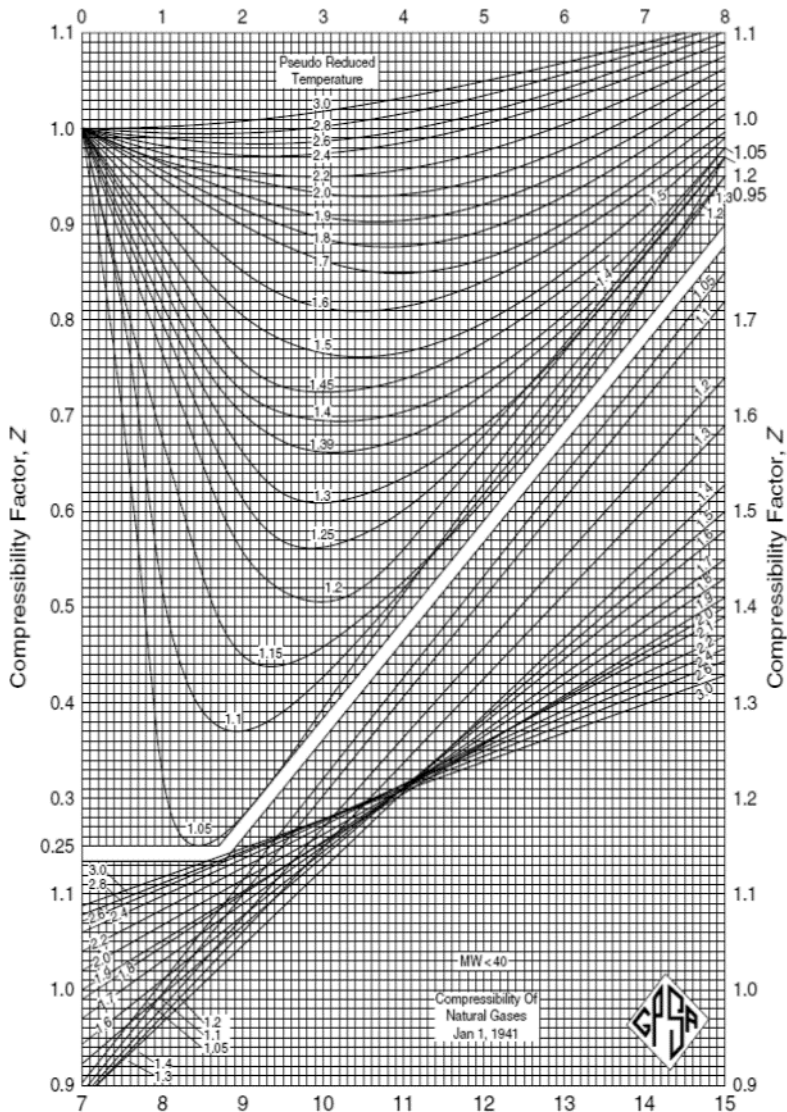
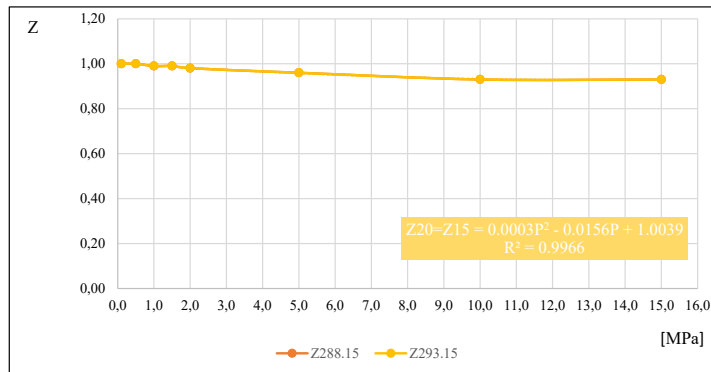


Figure 2. “Standing and Katz” nomogram for finding Supercompressibility Factor

Table 9. Table of Supercompressibility for 5% H₂

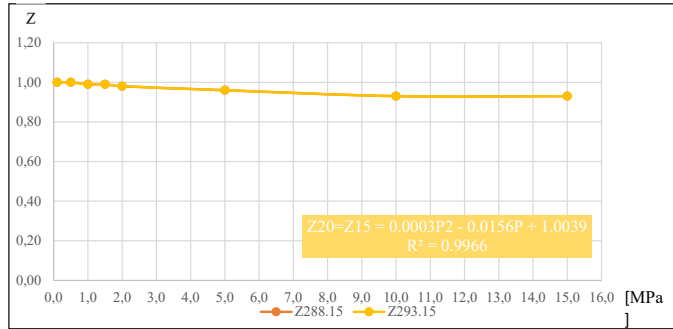
Table Z for 5% H ₂					
Pressure P [MPa]	P _{der}	T _{der} 288.15[K]	T _{der} 293.15 [K]	Z288.15	Z293.15
0.1	0.0225	1.5769	1.6042	1.00	1.00
0.5	0.1126	1.5769	1.6042	1.00	1.00
1.0	0.2252	1.5769	1.6042	0.99	0.99
1.5	0.3379	1.5769	1.6042	0.98	0.98
2.0	0.4505	1.5769	1.6042	0.97	0.97
5.0	1.1262	1.5769	1.6042	0.94	0.94
10.0	2.2524	1.5769	1.6042	0.89	0.89
15.0	3.3786	1.5769	1.6042	0.85	0.85



Graph 1. Z – Supercompressibility for 5% H₂

Table 10. Table of Supercompressibility for 15% H₂

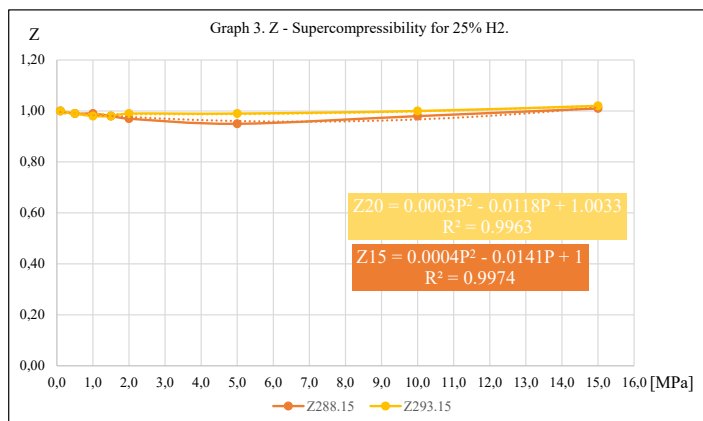
Table Z for 15% H ₂					
Pressure P [MPa]	P _{der}	T _{der} 288.15[K]	T _{der} 293.15 [K]	Z288.15	Z293.15
0.1	0.0243	1.7254	1.7553	1.00	1.00
0.5	0.1217	1.7254	1.7553	1.00	1.00
1.0	0.2434	1.7254	1.7553	0.99	0.99
1.5	0.3650	1.7254	1.7553	0.99	0.99
2.0	0.4867	1.7254	1.7553	0.98	0.98
5.0	1.2168	1.7254	1.7553	0.96	0.96
10.0	2.4336	1.7254	1.7553	0.93	0.93
15.0	3.6504	1.7254	1.7553	0.93	0.93



Graph 2. Z – Supercompressibility for 15% H₂

Table 11. Table of Supercompressibility for 25% H₂

Table Z for 25% H ₂					
Pressure P [MPa]	P _{der}	T _{der} 288.15[K]	T _{der} 293.15 [K]	Z288.15	Z293.15
0.1	0.0265	1.9048	1.9379	1.00	1.00
0.5	0.1323	1.9048	1.9379	0.99	0.99
1.0	0.2647	1.9048	1.9379	0.99	0.98
1.5	0.3970	1.9048	1.9379	0.98	0.98
2.0	0.5293	1.9048	1.9379	0.97	0.99
5.0	1.3233	1.9048	1.9379	0.95	0.99
10.0	2.6466	1.9048	1.9379	0.98	1.00
15.0	3.9698	1.9048	1.9379	1.01	1.02



Graph 3. Z – Supercompressibility for 25% H₂

From the data in Tables 9, 10, and 11 and Graphs 1, 2, and 3, we can see the dependence of the supercompressibility coefficient and the pressure.

At pressures and temperatures within the following ranges: $P = 0.1 \text{ MPa} \div 70.3 \text{ MPa}$; $T = 278 \text{ K} \div 511 \text{ K}$, the Lee-Gonzalez-Eakin relationship describes the change in viscosity of the gas-hydrogen mixture with sufficient accuracy. Formula 9 is used to calculate the viscosity of the gas-hydrogen mixture (Gerov, 2019).

$$\mu_g = A \times e^{B \times \rho_g^C} \quad (9)$$

Parameters A, B, C, and ρ_g are determined by the following dependencies (10-

$$A = \frac{(9.4 + 0.02 \times M_{gm}) \times (1.8 \times T)^{1.5}}{(209 + 19 \times M_{gm} + 1.8 \times T) \times 10^4} \quad (10)$$

$$B = 3.5 + \frac{547.77}{T} + 0.01 \times M_{gm} \quad (11)$$

$$C = 2.4 - 0.2 \times B \quad (12)$$

$$\rho_g = \frac{0.1202 \times P \times M_{gm}}{Z \times T} \quad (13)$$

Where:

μ_g – viscosity of the gas-hydrogen mixture [mPa.s]

M_{gm} – molar mass of the gas mixture [kg.kmol⁻¹]

Z – supercompressibility coefficient

P – the pressure at which the viscosity of the gas-hydrogen mixture is calculated [MPa]

T – the temperature at which the viscosity of the gas-hydrogen mixture is calculated [K]

Table 12. Viscosity of the gas-hydrogen mixture – μ

Viscosity of the gas-hydrogen mixture μ [mPa.s] (Lee-Gonzalez-Eakin)									
	T [K]	P [MPa]	Z288.15	Mg [kg. kmol ⁻¹]	A	B	C	ρ	μ [mPa.s]
5% H ₂	288.15	0.1	1.00	15.3417	0.01125	5.55441	1.28912	0.0006	0.01126
		0.5	1.00		0.01125	5.55441	1.28912	0.0032	0.01129
		1	0.99		0.01125	5.55441	1.28912	0.0065	0.01134
		1.5	0.98		0.01125	5.55441	1.28912	0.0098	0.01141
	T [K]	P [MPa]	Z293.15	Mg [kg. kmol ⁻¹]	A	B	C	ρ	μ [mPa.s]
	293.15	0.1	1.00	15.3417	0.01144	5.52198	1.29560	0.0006	0.01145
		0.5	1.00		0.01144	5.52198	1.29560	0.0031	0.01148
		1	0.99		0.01144	5.52198	1.29560	0.0064	0.01153
		1.5	0.98		0.01144	5.52198	1.29560	0.0096	0.01160
	T [K]	P [MPa]	Z288.15	Mg [kg. kmol ⁻¹]	A	B	C	ρ	μ [mPa.s]
15% H ₂	288.15	0.1	1.00	13.9390	0.01152	5.54038	1.29192	0.0006	0.01152
		0.5	1.00		0.01152	5.54038	1.29192	0.0029	0.01155
		1	0.99		0.01152	5.54038	1.29192	0.0059	0.01160
		1.5	0.99		0.01152	5.54038	1.29192	0.0088	0.01166
	T [K]	P [MPa]	Z293.15	Mg [kg. kmol ⁻¹]	A	B	C	ρ	μ [mPa.s]
	293.15	0.1	1.00	13.9390	0.01171	5.50796	1.29841	0.0006	0.01172
		0.5	1.00		0.01171	5.50796	1.29841	0.0029	0.01175
		1	0.99		0.01171	5.50796	1.29841	0.0058	0.01179
		1.5	0.99		0.01171	5.50796	1.29841	0.0087	0.01185
	T [K]	P [MPa]	Z288.15	Mg [kg. kmol ⁻¹]	A	B	C	ρ	μ [mPa.s]

25% H ₂	288.15	0.1	1.00	12.5363	0.01180	5.52635	1.29473	0.0005	0.01181
		0.5	0.99		0.01180	5.52635	1.29473	0.0026	0.01183
		1	0.99		0.01180	5.52635	1.29473	0.0053	0.01188
		1.5	0.98		0.01180	5.52635	1.29473	0.0080	0.01193
	T [K]	P [MPa]	Z293.15	Mg [kg.kmol ⁻¹]	A	B	C	ρ	μ [mPa.s]
	293.15	0.1	1.00	12.5363	0.01200	5.49393	1.30121	0.0005	0.01200
		0.5	0.99		0.01200	5.49393	1.30121	0.0026	0.01203
		1	0.98		0.01200	5.49393	1.30121	0.0052	0.01207
		1.5	0.98		0.01200	5.49393	1.30121	0.0079	0.01212

Result and discussion

Using the developed integrated model for determining the parameters of the reservoir rock when storing gas-hydrogen mixtures containing 5 to 25% hydrogen with sufficient accuracy for practical purposes, it is possible to determine the parameters of the gas-hydrogen mixture that determine the flow properties of the reservoir rock. The developed integrated model determines the change in the coefficient of supercompressibility, density, and viscosity at hydrogen concentrations ranging from 5 to 25% in a temperature range of 288.15 K to 293.15K and at pressures ranging from 0.1 MPa to 15 MPa. According to the calculations, the density of the gas-hydrogen mixture varies from 0.0306 to 0.0418 kg.m⁻³. It has been established that at 25% hydrogen, the coefficient of supercompressibility Z for the gas-hydrogen mixture is described by a different numerical model at a temperature of 288.15 K and 293.15 K in the pressure range from 0.1 to 15 MPa. The viscosity of the gas-hydrogen mixture with 5-25% hydrogen varies from 0.01126 to 0.01212 mPa.s.

Conclusions

In order to correctly determine the prospects and possibilities for storing gas-hydrogen mixtures in underground gas storage facilities and to analyze the processes occurring in the formation-bottomhole zone of the well, it is necessary to accurately determine the parameters of the gas-hydrogen mixture. This requires that the main processes occurring in the well-productive horizon system during the storage of gas-hydrogen mixtures be studied and analyzed for each specific site using the developed integrated model. The main processes occurring in the wellbore-productive horizon system depend on the amount of hydrogen in natural gas, which requires accurate determination of the parameters of the gas-hydrogen mixture. Correctly determining the processes occurring in the productive horizon is extremely important for determining whether to complete the well with a horizontal or vertical section (Georgiev, 2023). The data obtained on the parameters of the gas-

hydrogen mixture are extremely important for analyzing the influence of hydrogen on the capacity and flow parameters of the rock formation forming the productive horizon, at the bottomhole zone of the well, the influence of hydrogen during extraction and production on the production tubing column (PTC), and determining the optimal technological regime for injection and production of the gas-hydrogen mixture. The specified parameters of the gas-hydrogen mixture can be used in the design of hybrid heating systems (Karadjov, 2022).

Depending on the place of establishment, gas-hydrogen mixture storage facilities are divided into: underground gas storage in aquifers; underground gas reservoirs in depleted gas fields (Cavanagh et al., 2022), taking into account physical, chemical and energy aspects of underground hydrogen storage (Carden & Paterson, 1979).

Author Contribution

Veselin Mitkov conceived of the presented idea, designed the integrated model, adapted the theory and performed the calculations, and analyzed results, wrote the manuscript.

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NOTES

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