Geochemical Assessment of the Evolution of Groundwater under the Impact of Seawater Intrusion in the Mannar District of Sri Lanka

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NO. OF FIGURES: 4
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Text 1. Calculation of water parameters

The categorization of water hardness is based on $CaCO_3$ equivalents, where soft water registers below 75 mg/L as $CaCO_3$. Slightly hard water falls within the range of 75 to 150 mg/L as $CaCO_3$, while moderately hard water encompasses concentrations between 150 and 300 mg/L as $CaCO_3$. Water is classified as very hard when the values surpass 300 mg/L as $CaCO_3$, according to the classification by Sawyer and McCarty in 1967 [1].

The calculation of hardness is based on the following equation in equivalent of $CaCO_3$ mg/L.

Hardness [mg/L] = 2.497 [Ca, mg/L] + 4.118 [Mg, mg/L]

Alkalinity is the acid-neutralizing capacity due to the presence of HCO_3^-, CO_3^{2-} and hydroxide OH^- ions of the water. The total alkalinity was determined by H_2SO_4 (0.01N) titration with methyl orange as the indicator. $[HCO_3^-]$ is calculated using the following equation.

$[HCO_3^-]$ = 1.22 × (Total Alkalinity/mg/L)

The concentrations in terms of milliequivalents per liter (meq/L) is used to measure the chemical activity of ions in a solution, providing a standardized approach to convey the quantity of substances involved in various chemical reactions.

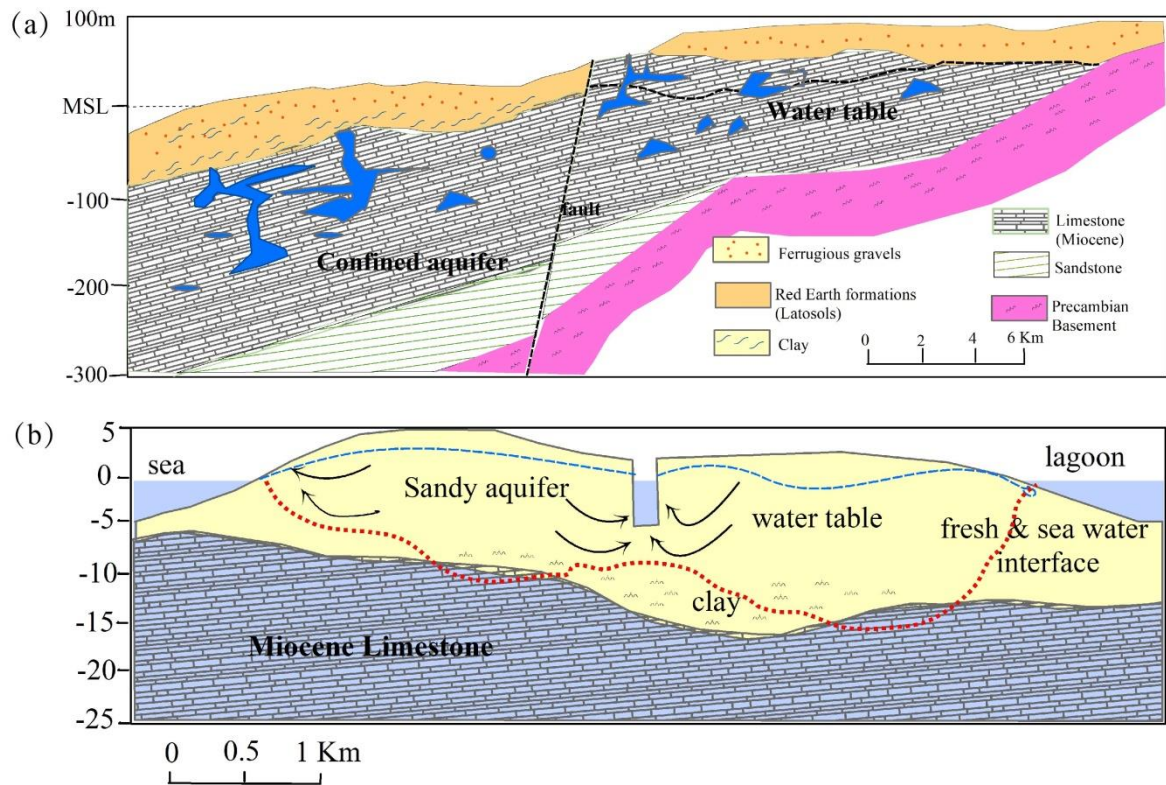$$meq = \frac{mg \times Valence}{Molecular\ weight}$$

Figure S1. East-West geological schematic cross sections of (a) deep confined aquifer basin system of Mannar mainland [2] and (b) sandy aquifer systems of Mannar Island [3]
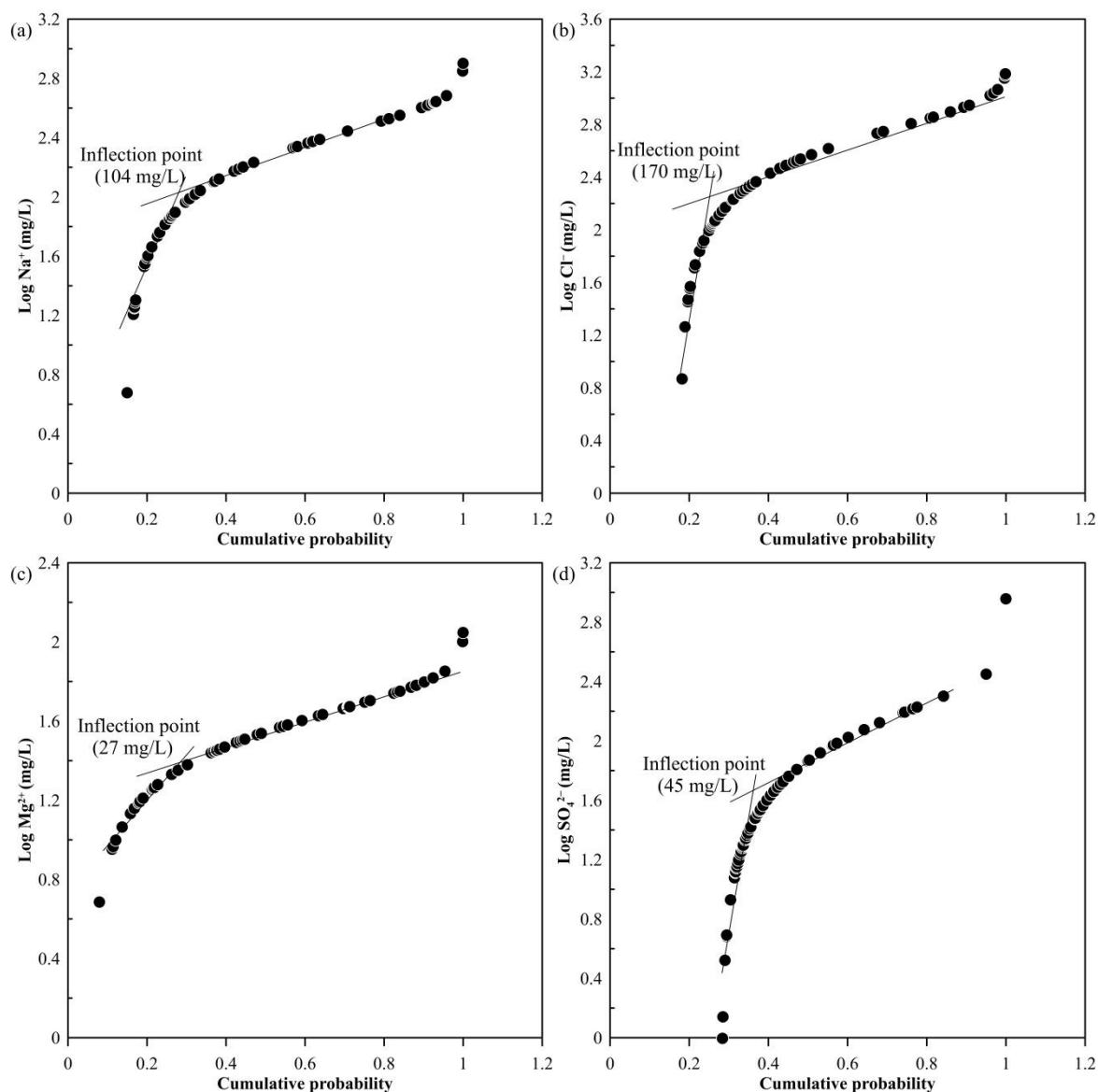
Figure S2. Cumulative probability (%) for calculating the threshold value of critical parameters (Na^+, Mg^{2+}, Cl^-, SO_4^{2-})
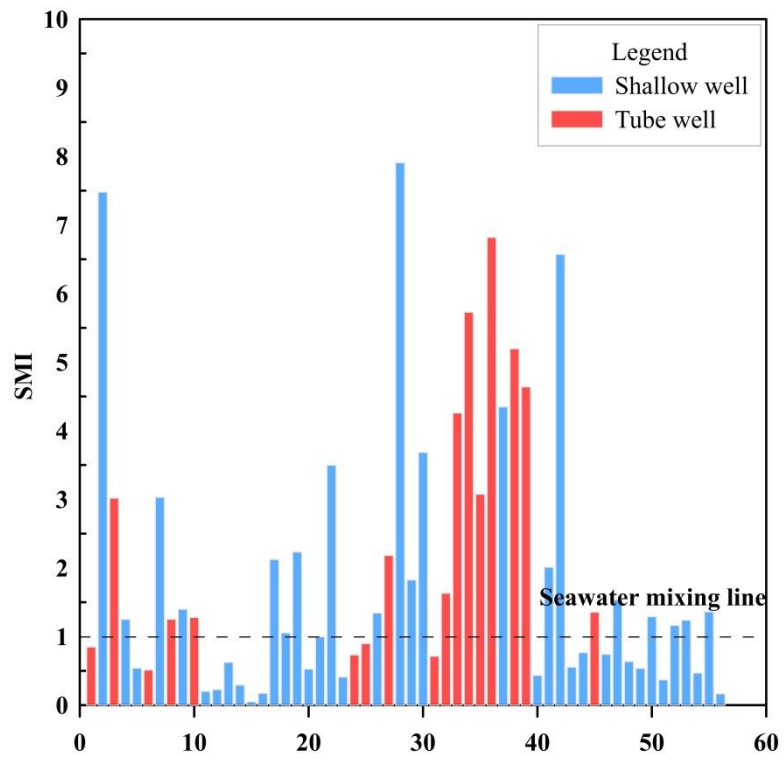
Figure S3. SMI values of groundwater in Mannar district.
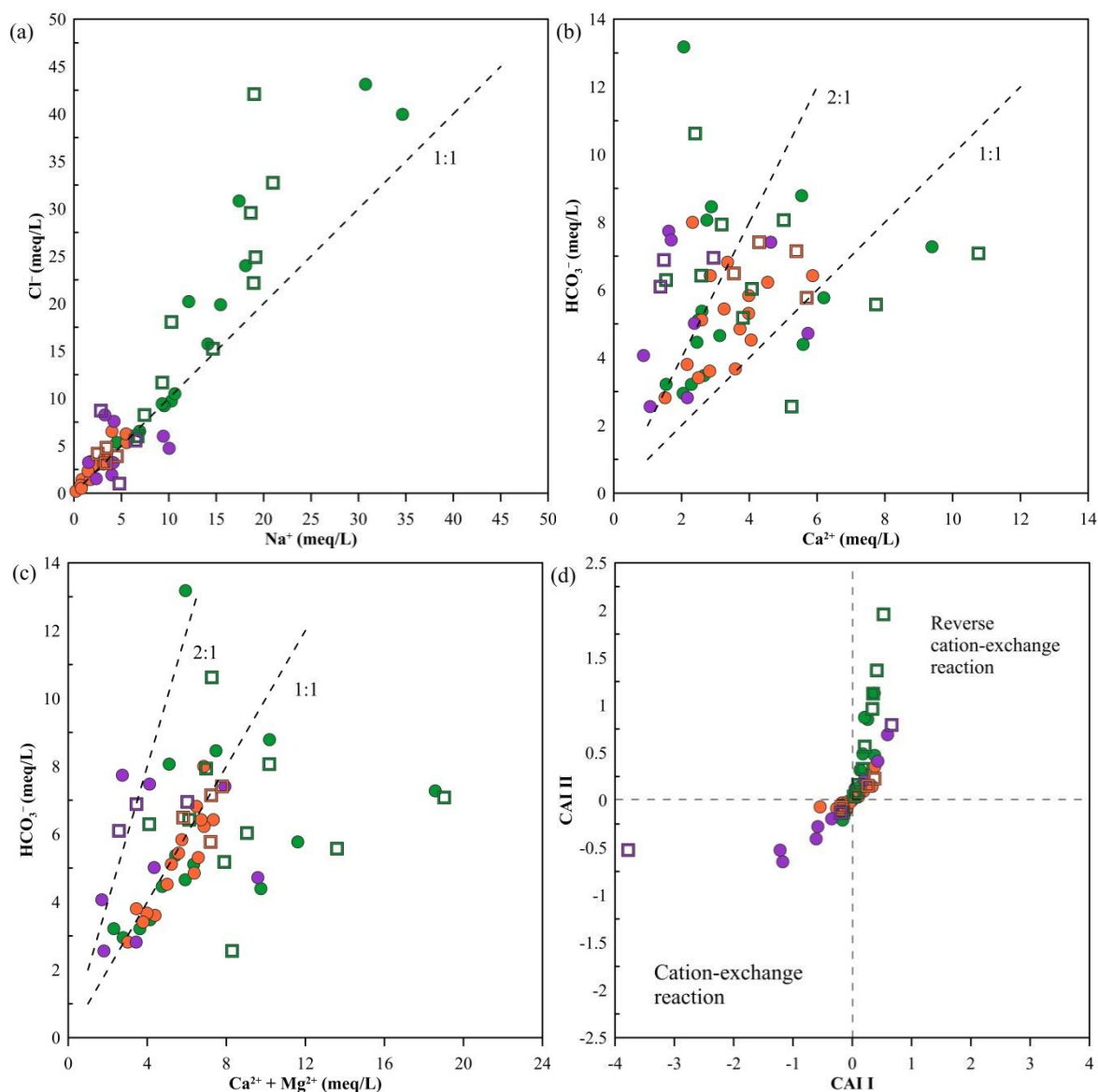
Figure S4: Hydrochemical relationships between ions. Orange, green, and purple colors represent HCO_3-Ca type, Cl-Na type, and Mixed type, respectively. Solid and hollow points correspond to shallow well and tube well groundwater, respectively. (a) Cl^- vs Na^+. (b) HCO_3^- vs Ca^{2+}. (c) HCO_3^- vs $(Ca^{2+} + Mg^{2+})$. (d) chloro-alkaline index diagram CAI II vs CAI I.

Table S1. The statistic of groundwater geochemical compositions.

Indices	Unit	Minimum	Maximum	Average	SLS 614-2013	WHO 2017
pH		5.89	7.97	6.82	6.5 - 8.5	6.5 - 8.5
Temperature	°C	27.3	28.2	27.6	-	-
EC	µS/cm	384	5910	1787	750	750
TDS	mg/L	192	2950	894	500	500
Na^+	mg/L	4.77	797.00	184.03	250	200
K^+	mg/L	0.29	68.01	15.24	-	-
Mg^{2+}	mg/L	4.85	111.55	35.07	-	-
Ca^{2+}	mg/L	17.54	215.23	70.72	-	-
HCO_3^-	mg/L	156	804	354	200	-
F^-	mg/L	0.14	2.48	0.69	1.0	1.5
Cl^-	mg/L	7.38	1530.69	369.54	250	250
Br^-	mg/L	<0.01	5.5	1.2	-	2
NO_3^-	mg/L	<0.01	85.6	8.1	50	50
SO_4^{2-}	mg/L	0.99	906.70	73.19	200	200
Total Hardness	mg/L	84.8	950.8	321.0	250	-
DOC	mg/L	0.59	15.16	5.82	-	-

Table S2. Relative weight of chemical parameters with threshold values.

Parameter	Threshold values (S_i)	Weight (w_i)	Relative Weight (Wi)
pH	6.5–8.5	4	0.105263
Dissolved oxygen	5	5	0.131579
Total Dissolved solids	500	4	0.105263
Alkalinity	200	2	0.052632
Electrical conductivity	750	5	0.131579
Na^+	200	1	0.026316
Ca^{2+}	75	2	0.052632
Mg^{2+}	50	2	0.052632
F^-	1.5	2	0.052632
Cl^-	250	3	0.078947
SO_4^{2-}	200	4	0.105263
NO_3^-	50	4	0.105263
		$\sum w_i = 38$	$\sum W_i = 1.0000$

Table S3. Sub-stages (in %) in freshening and intrusion phases

	HFs	Sub-stage	Cation exchange evaluation	Percentages (%)	Percentages (%)
Shallow wells	NaCl	f_1		15.4	
	NaMixCl	f_2		5.1	
	NaMixHCO$_3$, MixNaMixHCO$_3$	f_3	freshening	5.1	74.36
	NaHCO$_3$, CaHCO$_3$, MixNaHCO$_3$,MixCaHCO$_3$	f_4 + FW		48.8	
	MixNaMixCl, MixCaMixCl	i_2		5.1	
	MixNaCl, MixCaCl	i_3	intrusion	5.1	25.64
	NaCl	i_4 + SW		15.4	
Tube wells	NaCl	f_1		23.4	
	NaMixHCO$_3$	f_3	freshening	6.0	64.7
	NaHCO$_3$, CaHCO$_3$, MixNaHCO$_3$, MixCaHCO$_3$	f_4 + FW		35.3	
	NaCl	i_4 + SW	intrusion	35.3	35.3

References

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