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International Baccalaureate Extended Essay

Chemistry

How do the concentration of sodium chloride in aqueous solution and the pH of a solution affect their absorption by diaper gel, sodium polyacrylate?

Candidate number:

Examination session: May 2012

Word count: 3999 ✓!

Supervisor:

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Abstract

This essay investigates how the concentration of sodium chloride in aqueous solution and the pH of a solution affect their absorption by diaper gel, sodium polyacrylate. In a self-designed experimental procedure, solutions of various concentrations of sodium chloride were made and added to samples of sodium polyacrylate extracted from diapers. The amount of solution absorbed by the gel was recorded by separating the unabsorbed solution from the gel by centrifugation, and evaporation in an oven. The procedure was repeated, this time with solutions of different pH made by the dilution of hydrochloric acid or sodium hydroxide. Here, the separation of the absorbed and unabsorbed solutions was done using gravimetric filtration. After data processing and translation of data into absorption factors – the number of times its own weight that the sodium polyacrylate can absorb – several conclusions have been drawn. It was found that as the concentration of sodium chloride increases, the sodium polyacrylate absorbs less solution, as the increasing amount of sodium cations in the solution hinders the hydrogen bonding that allows water molecules to attach to the polymer chain. It was also found that low pH values cause low absorption by the sodium polyacrylate, as the same can be said for the hydrogen cations from the acid solution. Conversely, with a solution of distilled water (includes no sodium chloride), absorption immediately rises. The same can be said for the pH experiment when pH rises to neutral and basic values. Results were compared with theoretical models, and improvements to the procedure suggested. They include the use of successive gravimetric filtrations instead of centrifugation to separate the gel from the unabsorbed solution in the sodium chloride experiment, and the use of industrially prepared solutions of appropriate pH to use as samples for solutions of different pH.

Word count: 297

1. Introduction

Modern chemistry has brought to the world a type of material that has transfigured everyday life: gel. This paper provides a study on a specific variety of gel called a *hydrogel*, whose characteristic property is to expand under the presence of water, due to a network of hydrophilic polymer chains. The first man-made hydrogels were introduced in the 1960s, when American scientists established a gel of granular consistency to retain water in soils¹. Hydrogels can contain up to more than 99% water² without dissolving, and are permeable to oxygen and other nutrients³, rendering them useful for many applications. Referred to as “superabsorbent polymers”, their uses range from contact lenses to medical tissue engineering, hairgels, or diapers. This essay aims to investigate two properties of the hydrogel found in diapers, known as *sodium polyacrylate*, a partially neutralized form of prop-2-enoic acid officially known as *sodium prop-2-enoate*, bearing the chemical formula $[C_3H_3NaO_2]_{n(s)}$, more precisely $[CH_2CHNaOO]_{n(s)}$, with a main $[COONa]$ functional group. This functional group qualifies sodium polyacrylate as a salt of a carboxylic acid, in this case prop-2-enoic (acrylic) acid, $CH_2CHCOOH$. Sodium polyacrylate is considered an anionic polymer, as the dissociation of the Na^+ and O^- ions when in contact with aqueous solutions leaves lone oxygen anions on the polymer chain. Its structure is shown on the next page.

¹ M² POLYMER TECHNOLOGIES. *History of Super Absorbent Polymer Chemistry*. URL: http://www.m2polymer.com/html/history_of_superabsorbents.html [13 July 2011].

² SOCIETY FOR BIOMATERIALS. *Biomaterial of the month: Hydrogels*. URL: <http://www.biomaterials.org/week/bio17.cfm> [12 July 2011].

³ K.T. NGUYEN; J.L. WEST. *Photopolymerizable hydrogels for tissue engineering applications*. *Biomaterials*, No. 23. 2002.

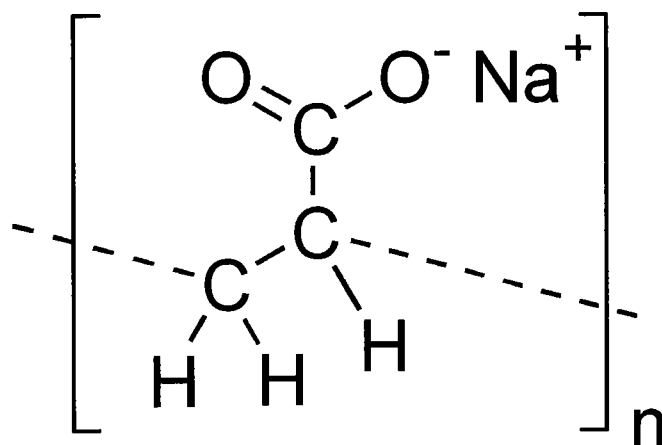


Fig. 1 Structure of a sodium polyacrylate repeat unit⁴

Sodium polyacrylate is produced by neutralizing the carboxyl group in polymerized acrylic acid, $[CH_2CHCOOH]_{n(aq)}$, with sodium hydroxide, as shown below.

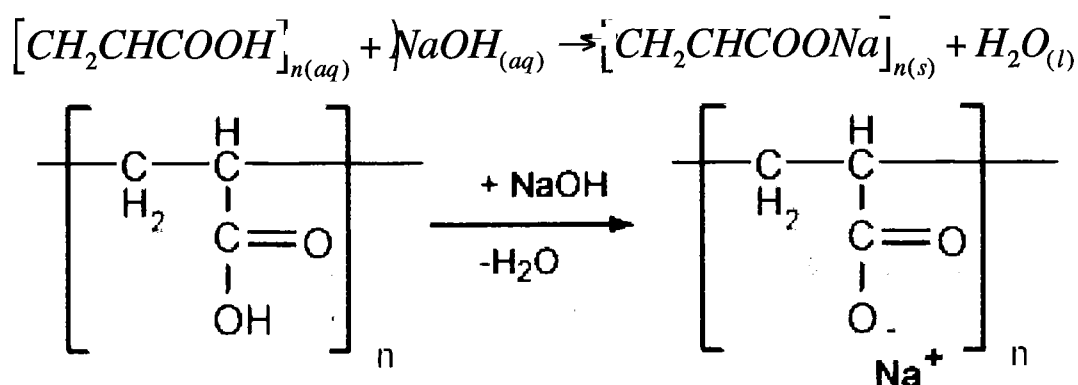


Fig. 2 Manufacture of sodium polyacrylate (equation and diagram)⁵

Diaper manufacturers claim that sodium polyacrylate can absorb hundreds of times its weight in distilled water⁶, but two listed properties of the polymer are sensitivity to varying pH and to the presence of electrolytes in a solution it is put in contact with. These characteristics effectively are two differences between water and urine.

⁴ WIKIMEDIA COMMONS. *Sodium polyacrylate*. URL: http://commons.wikimedia.org/wiki/File:Sodium_polyacrylate.png [12 July 2011].

⁵ INKLINE GREECE. *Dispersing process*. URL: <http://www.inkline.gr/inkjet/newtech/tech/dispersion/> [12 July 2011].

⁶ EVONIK INDUSTRIES. *About superabsorbents*. URL: <http://www.superabsorber.com/product/superabsorber/en/about/favor/pages/default.aspx> [13 July 2011].

When sodium polyacrylate is placed in water, cross-links form between polyacrylate chains. Cross-links are chemical bonds connecting polymer chains, forming a three-dimensional structure that strengthens the chains⁷, decreasing the system's entropy. They form here, as the only major intermolecular force present is hydrogen bonding with water molecules, as shown below.

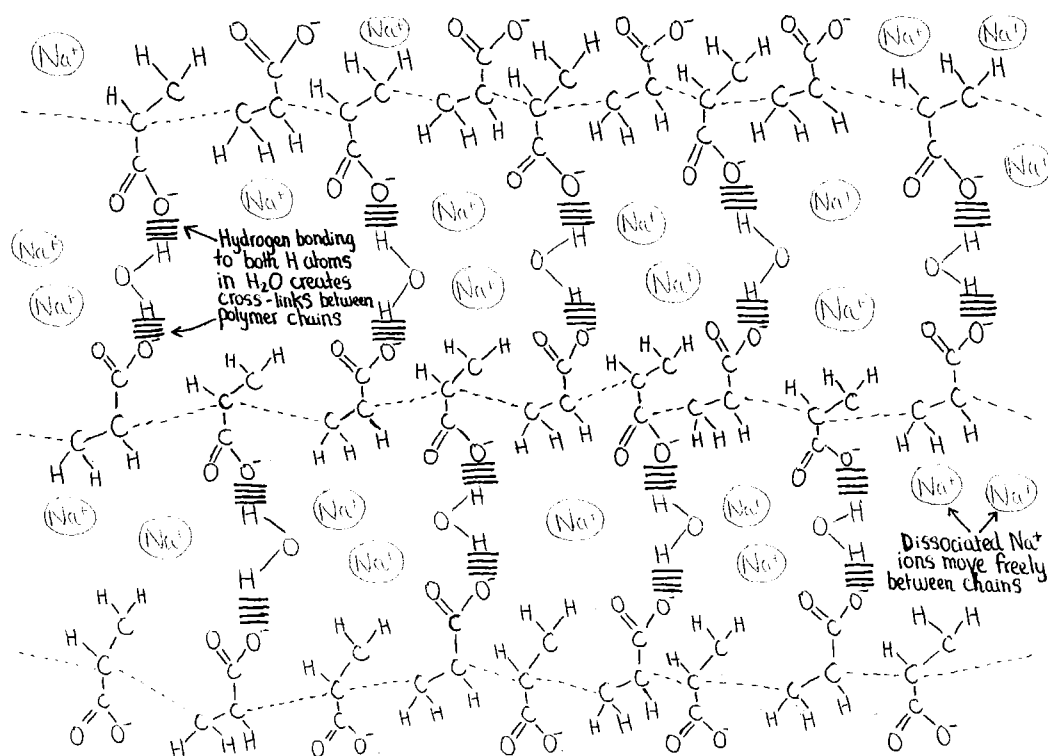


Fig. 3 Cross-link formation between sodium polyacrylate molecules

This hydrogen bonding is possible since the Na^+ ions from sodium polyacrylate, when in contact with water, detach themselves by the process of osmosis (spreading out evenly between the polymer and the surrounding solution), leaving negatively charged carboxylate groups (R-COO^-) behind. The repulsion between the negative charges results in the uncoiling of the polymer chain⁸, which then interacts more readily with water molecules, as shown on the next page.

⁷ NEUSS, Geoffrey. *IB Study Guides, Chemistry Standard and Higher Level, Second Edition*. Oxford: Oxford University Press, 2007. 186 pages.

⁸ UNIVERSITY OF ILLINOIS. *WaterCAMPWS: Superabsorbent Polymers*. URL: [http://www.watercampws.uiuc.edu/waterclear/labs/original labs/polymer lab/Superabsorbent%20Polymers.pdf](http://www.watercampws.uiuc.edu/waterclear/labs/original%20labs/polymer%20lab/Superabsorbent%20Polymers.pdf) [26 October 2011].

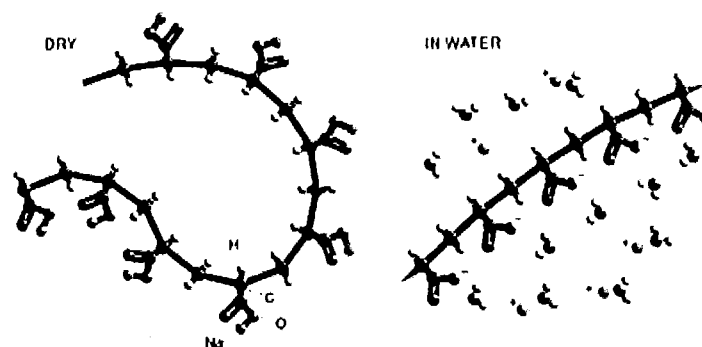


Fig. 4 Representation of the uncoiling of the polyacrylate chain in water⁹

Likewise, water molecules move towards the chain by osmosis and form intermolecular bonds with its oxygen anions forsaken by the sodium cations, forming cross-links, resulting in the swelling of the solution, and an increase in viscosity. This explains the hydrophilic behavior of sodium polyacrylate. Once cross-links are formed, the polymer reaches equilibrium with the water surrounding it, as shown below.

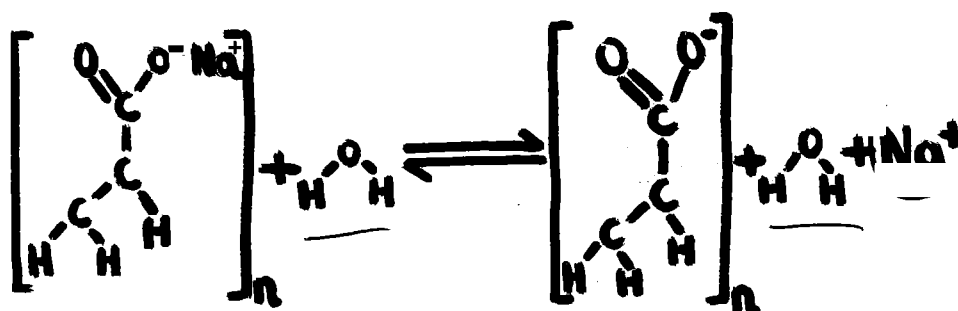


Fig. 5 Representation of the equilibrium between sodium polyacrylate and water

With reference to Fig. 5, a difference in pH or the presence of electrolytes in the solution could disrupt the equilibrium, as new reagents would be present, thus altering the polymer's superabsorbent capacities. This essay attempts to investigate these two factors. Indeed, diapers are designed to absorb urine, which contains about 0.9% of salt¹⁰ and has a variable pH (normal values span from 4.6 to 8.0)¹¹, rather than distilled water. The puzzling properties of

⁹ THE DIAPER INDUSTRY SOURCE. *What are the components of a typical disposable diaper?* URL: <http://www.disposablediaper.net/faq.asp?1> [13 July 2011].

¹⁰ THE DIAPER INDUSTRY SOURCE. *Ibidem*.

¹¹ MEDLINEPLUS. *Urine pH*. URL: <http://www.nlm.nih.gov/medlineplus/ency/article/003583.htm> [13 July 2011].

superabsorbent polymers, and the fact that the flourishing polymer industry is increasingly shaping modern life, in domains ranging from medicine to industrial and household applications, make an investigation of sodium polyacrylate worthy. Moreover, it addresses a revolutionary product of modern chemistry in that it has allowed the advent of the modern diaper and the boom of the contact-lens industry. The research question is as follows:

How do the concentration of sodium chloride in aqueous solution and pH of a solution affect their absorption by diaper gel, sodium polyacrylate?

For this investigation, an experimental procedure was designed entirely from scratch, using apparatus available in the school laboratory. Indeed, previous methods have been established for this sort of experiment, but all require very advanced apparatus only available in university laboratories. For instance, a method using microvalves (1000×180µm cross-sections) to measure the one-dimensional swelling/expansion of sodium polyacrylate¹² seems compelling, but can simply not be reproduced in high school laboratories.

The independent variables in the experiment can be identified as sodium chloride concentration and pH, and the dependent variable as the amount of solution absorbed by the sodium polyacrylate. The variable suspect to altering results, temperature, will be controlled by making sure all experiments are conducted at uniform temperature (between 25-26°C), and monitoring each solution's temperature. The other controlled variables are the mass of sodium polyacrylate crystals per sample and the volume of solution reacted.

Literature indicates a linear relationship between sodium chloride concentration and sodium polyacrylate absorption, however for concentration 0.0 mol dm⁻³ (water), absorption rises substantially¹³. The relationship is sketched overleaf.

¹² S. K. DE; D. J. BEEBE; N. R. ALURU; B. JOHNSON; W. C. CRONE; J. MOORE. *Equilibrium swelling and kinetics of pH-responsive Hydrogels: Models, Experiments, and Simulations*. Journal of microelectromechanical systems, Vol. 11, No. 5. October 2002.

¹³ K. KABIRI; H. OMIDIAN; S.A. HASHEMI; M.J. ZOHURIAAN-MEHR. *Synthesis of fast-swelling superabsorbent hydrogels: effect of crosslinker type and concentration on porosity and absorption rate*. European Polymer Journal, Vol. 39, Issue 7. 2003.

Aqueous NaCl concentration vs. Mass of solution absorbed

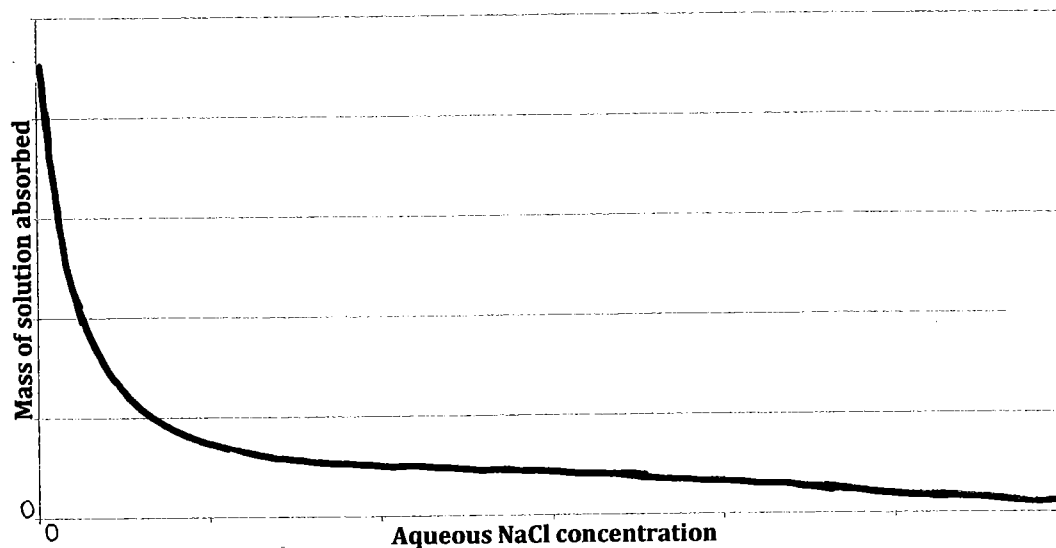


Fig. 6 Theoretical model: aqueous NaCl concentration against absorption of gel

For the second experiment, acidic pH values are expected to yield small and slowly increasing amounts of solution absorbed, which substantially increases somewhere between pH 6.0 and 7.0 (theoretical pH of distilled water). Above this value, absorption stabilizes.¹⁴ The relationship is sketched below.

pH of solution vs. Mass of solution absorbed

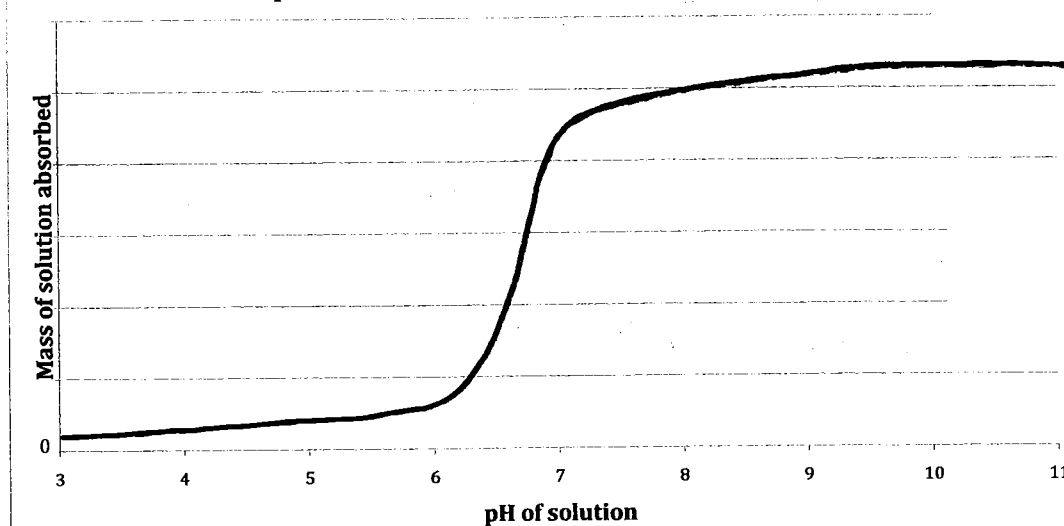


Fig. 7 Theoretical model: pH of solution against absorption of gel

¹⁴ S. K. DE; D. J. BEEBE; N. R. ALURU; B. JOHNSON; W. C. CRONE; J. MOORE. *Opus citatum*.

2. Method

Refer to Appendix I for list of apparatus.

1. Production of standard saturated sodium chloride solution¹⁵

Using solubility curves, the solubility of sodium chloride in water was determined at 36.60g/100g, at the recorded water temperature of 23.5°C¹⁶. Known amounts of excess salt (for some to remain non-dissolved) were placed in two 2000cm³ beakers, and then filled with distilled water up to the 1400cm³ and 1600cm³ marks respectively. Both beakers and their contents were magnetically stirred overnight. Leftovers were gravimetrically filtered the next day, put to dry at 80°C in an oven, and weighed to then find the amount of salt dissolved. The solution's concentration was calculated with this data. This saturated solution was stored in a 3000cm³ standard flask. Note: It was found, and verified, that the experimental solubility of the salt was significantly inferior to literature values.

2. Dilution of saturated solution into samples of different concentration

Once its concentration was found, samples of the standard solution were diluted with distilled water in 100cm³ graduated cylinders, with the help of dropping pipettes, to obtain twelve 100cm³ samples of concentrations:

-Saturated	-2.5 moldm ⁻³
-5.0 moldm ⁻³	-2.0 moldm ⁻³
-4.5 moldm ⁻³	-1.5 moldm ⁻³
-4.0 moldm ⁻³	-1.0 moldm ⁻³
-3.5 moldm ⁻³	-0.5 moldm ⁻³
-3.0 moldm ⁻³	-0.0 moldm ⁻³ (H ₂ O(l))

Cylinders were sealed with rubber corks to prevent evaporation.

¹⁵ Details (irrelevant to the development of this essay) on this step are found in Appendix II.

¹⁶ P.W. ATKINS; J.A. BERAN. *General Chemistry, Second Edition*. New York: Scientific American Books, 1992. 922 pages.

3. Dilution of acid and base into samples of different pH¹⁷

Since 0.1mol dm^{-3} hydrochloric acid has a pH of 1 and 0.1mol dm^{-3} sodium hydroxide has a pH of 13, samples of both solutions were serially diluted with distilled water in 100cm^3 graduated cylinders with the help of dropping pipettes, to obtain 100cm^3 samples of pH 3.0, 4.0, 5.0, 6.0 (from hydrochloric acid), 7.0 (neutralized solution), 8.0, 9.0, 10.0, 11.0, (from sodium hydroxide). For each sample the pH was verified with a pH probe calibrated with pH 4.0 and 7.0 (for acid range), and 7.0 and 10.0 (for alkaline range) buffer solutions. The cylinders were sealed with rubber corks.

4. Extraction of sodium polyacrylate from diapers

One¹⁸ disposable "HUGGIES Little Walkers Step-in nappy" was carefully opened, using scissors to cut the cellulose enclosing the gel pocket. The sodium polyacrylate crystals were extracted over a sheet of paper, and the cellulose stuck to the crystals removed with a scalpel. Once the crystals were extracted, they were placed on weighing boats and weighed into twenty-three $0.15\text{g}(\pm 0.01)$ samples.

5. Reaction of sodium polyacrylate with aqueous sodium chloride and different pH samples

Two test trials were conducted to ensure that solutions of 100cm^3 distilled water and pH 7.0 respectively would not be entirely absorbed by 0.15g of gel crystals¹⁹. Each 100cm^3 sodium chloride solution was then transferred into a

¹⁷ Details (irrelevant to the development of this essay) on this step are found in Appendix III.

¹⁸ One diaper contains about 10 grams of SAP, which is more than enough to extract twenty-three 0.15g samples and two others for trial runs.

¹⁹ This fixed amount has been determined so that it will never absorb an entire 100cm^3 distilled water sample, predicted to absorb the most by literature. Since the water weighs 100g , a mass of polymer under $\frac{100}{500} = 0.2\text{g}$ is needed. The weight of gel samples has then been fixed at 0.15g .

250cm³ beaker. Twelve of the 0.15g samples of sodium polyacrylate were introduced into each solution. About 10-12 minutes were left to ensure that the crystals swelled to a maximum. Part of the unabsorbed solution was then drained into a waste beaker, making sure no gel was lost. The rest of the beakers' contents were each time poured into four centrifuge tubes (total capacity 50cm³)²⁰ initially weighed empty, making sure all the gel was transferred. The tubes were placed in a centrifuge machine for 2 minutes at 4000rpm to separate the gel from the unabsorbed solution. The separated solution was again drained, being careful not to lose any gel. The tubes were partially dried overnight in the oven at 50°C, then dried at room temperature, so that symbolical leftovers of unabsorbed solution would evaporate. The tubes, with only swollen gel left, were weighed the next day. The difference was then made between their empty weight and the weight with the swollen gel and the initial mass of the gel crystals, to calculate the amount of solution absorbed. Note that for the distilled water sample, according to literature, the crystals will have swollen too much for all the gel to be transferred into four centrifuge tubes. For this trial, the beaker's content was placed in a sieve - another separation technique - that was subsequently placed in the oven with the tubes.

This step was repeated, with the nine remaining samples of sodium polyacrylate introduced into each solution of different pH. Here, the separation method used was gravimetric filtration of the gel using funnels in Erlenmeyer flasks, and very impermeable Whatman Number 1 filter paper. The gel and paper were dried in the same manner as the sodium chloride.

Note: Hydrochloric acid and sodium hydroxide should be handled cautiously as they are corrosive, and sodium polyacrylate should not be inhaled (irritant).

²⁰ At least 50cm³ of unabsorbed solution could always be removed (excl. 0.0mol dm⁻³ sample).

3. Results

The experimental results are presented in tabular form, and relevant data expressed graphically in order to analyze relevant relationships. With the help of graphs, the theoretical absorption of the polymer with a solution of 0.9% sodium chloride (salinity of urine), expected to drop to about 30 times its own weight²¹, will be verified, as well as the variation in absorption that urine pH brings. Calculations determining the factor of the sodium polyacrylate's own weight absorbed are also included.

Sample number	Concentration of sample / moldm ⁻³	Mass of empty centrifuge tubes / g	Mass of centrifuge tubes with hydrated solution / g	Mass of gel crystals / g	→ Mass of absorbed solution ²² / g
1.1	5.1 (saturated)	N/A	N/A	0.15	N/A
1.2	5.0	N/A	N/A	0.15	N/A
1.3	4.5	N/A	N/A	0.15	N/A
1.4	4.0	N/A	N/A	0.15	N/A
1.5	3.5	N/A	N/A	0.15	N/A
1.6	3.0	57.97	59.33	0.15	1.21
1.7	2.5	49.12	51.42	0.15	2.15
1.8	2.0	49.08	51.68	0.15	2.45
1.9	1.5	49.14	52.05	0.15	2.76
1.10	1.0	49.14	52.17	0.15	2.88
1.11	0.5	49.21	52.94	0.15	3.58
1.12	0.0 (water)	N/A	N/A	0.15	23.62
Uncertainty	<i>±0.1²³</i>	<i>±0.01</i>	<i>±0.60</i>	<i>±0.01</i>	<i>±0.60</i>

Table 1 Numerical data from the experiment involving sodium chloride concentration, leading to calculation of the mass of solution absorbed

Observations: The first five samples tested yielded virtually inexistent amounts of swollen gel. It took about 7-10 minutes for gels in the beakers to stabilize their expansions (i.e. reach equilibrium).

²¹ K. KABIRI; H. OMIDIAN; S.A. HASHEMI; M.J. ZOHURIAAN-MEHR. *Op. cit.*

²² Equal to: mass of tubes with hydrated sol. – mass of crystals – mass of empty tubes. Since this is a subtraction, uncertainties of the three terms are added and rounded to one significant figure.

²³ Uncertainties in italic are rounded uncertainties cumulated from all measuring apparatus that the material has been in contact with.

Sample number	pH of sample ²⁴	Mass of filter paper / g	Mass of filter paper and hydrated solution / g	Mass of gel crystals / g	Mass of absorbed solution / g
2.1	3.00	1.55	2.81	0.15	1.26
2.2	4.00	1.57	3.03	0.15	1.46
2.3	5.00	1.56	2.76	0.15	1.20
2.4	6.00	1.54	3.25	0.15	1.71
2.5	7.00 (neutral)	1.56	6.10	0.15	4.54
2.6	8.00	1.55	5.98	0.15	4.43
2.7	9.00	1.57	6.43	0.15	4.86
2.8	10.00	1.56	6.29	0.15	4.73
2.9	11.00	1.56	6.36	0.15	4.80
Uncertainty	±0.20	±0.01	±0.50	±0.01	±0.50

Table 2 Numerical data from the experiment involving pH, leading to calculation of the mass of solution absorbed

Observations: It took about 7-11 minutes for the gels to reach equilibrium.

The graph below expresses the relevant content found in Table 1.

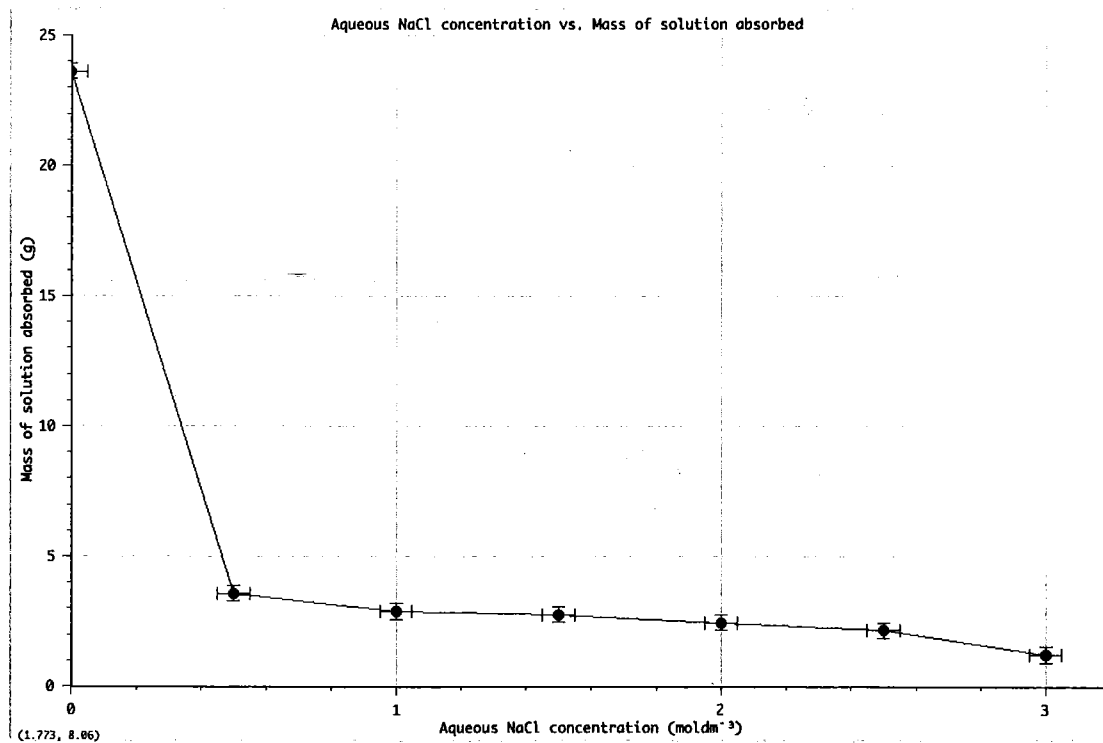


Fig. 8 Graph plotting NaCl_(aq) concentration against mass of solution absorbed

²⁴ Uncertainty in pH is a propagation of the uncertainties of the pH-meter, the buffer solutions and their measured pH, and the quantities of acid and base involved in the serial dilution.

The graph on the previous page supports the predicted relationship. Effectively, even a symbolical concentration of sodium chloride significantly alters the absorption of sodium polyacrylate. The graph below expresses the variation within solutions that include sodium chloride (distilled water sample is ignored).

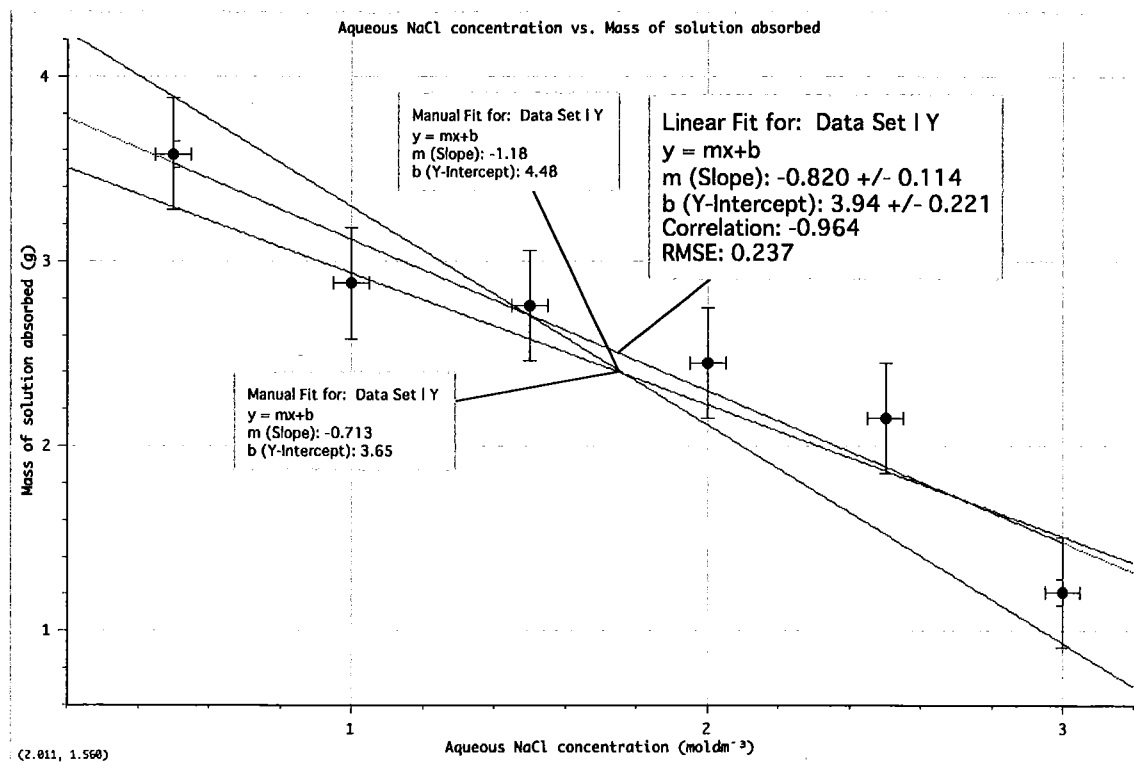


Fig. 9 Graph plotting aqueous sodium chloride concentration against mass of solution absorbed (excluding 0.0 mol dm^{-3} sample)

The graph above supports the prediction that there is a linear relationship between concentration of aqueous sodium chloride and amount of solution absorbed by sodium polyacrylate. The linear fit plotted with respect to the data points fits into each of the error bars, validating the results. The x-intercept can be calculated at about 4.8 mol dm^{-3} , meaning that beyond this concentration, no solution would be theoretically absorbed.

The graph on the next page shows how sodium polyacrylate's absorption varies with respect to difference in pH.

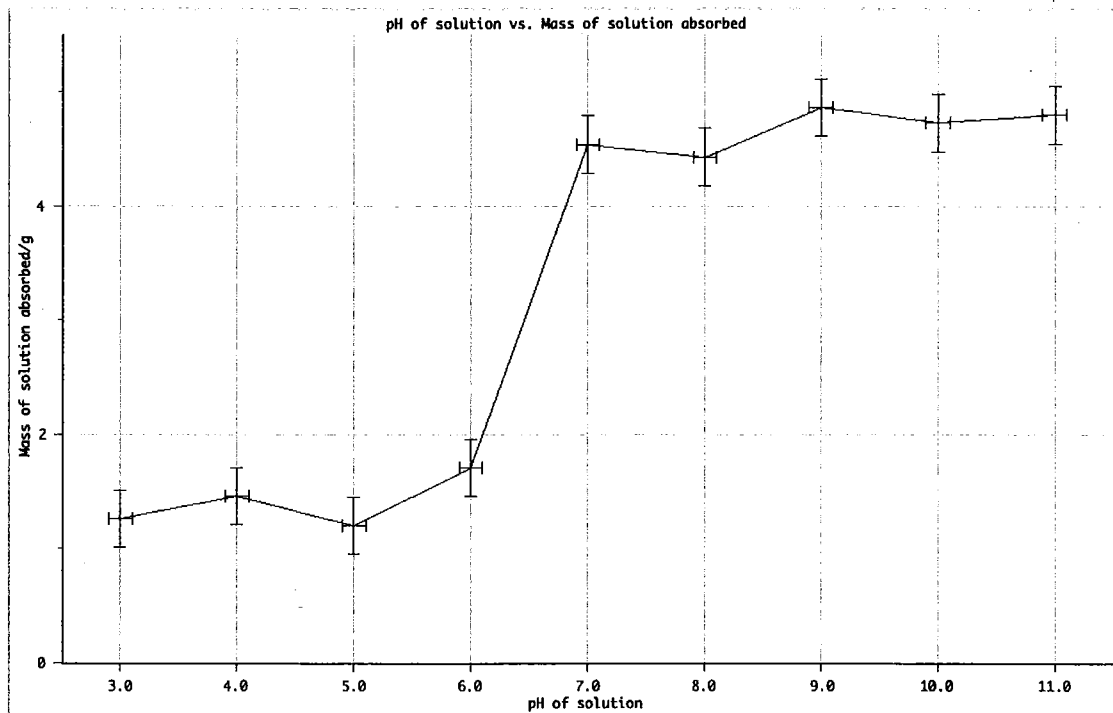


Fig. 10 Graph plotting pH of solution against mass of solution absorbed

The graph supports the prediction in Fig. 7.

Using the formula below, the factor of the crystals' weight that has been absorbed can be calculated:

$$\frac{\text{mass}_{\text{absorbed}}}{\text{mass}_{\text{crystals}}}$$

For instance, for the 3.0 mol dm^{-3} sodium chloride sample:

$$\frac{1.21}{0.15} \approx 8.07 \quad \text{This sample absorbed about 8.07 times its own weight.}$$

The factors are tabulated in the two following tables.

Sample number	Concentration of sample / moldm ⁻³	Absorption factor
1.1	5.13(saturated)	N/A
1.2	5.00	N/A
1.3	4.50	N/A
1.4	4.00	N/A
1.5	3.50	N/A
1.6	3.00	8.07 (±6.00)
1.7	2.50	14.30 (±7.00)
1.8	2.00	16.30(±7.00)
1.9	1.50	18.40 (±8.00)
1.10	1.00	19.20 (±8.00)
1.11	0.50	23.90 (±9.00)
1.12	0.00 (H ₂ O(l))	157.00 (±35.00)
Uncertainty	±0.10	Individual ²⁵

Table 3 Factor of their own weight that sodium polyacrylate crystals have absorbed with varying concentration of sodium chloride in aqueous solution

The absorption factor of distilled water is about 157 times its own weight, a percentage error of $\frac{500 - 157}{500} \times 100 = 68.6\%$ compared to the expected value of 500. This error is not encompassed by the uncertainty.

It is hard to calculate a value for the absorption factor of 0.9% aqueous sodium chloride ($\approx 0.15 \text{ moldm}^{-3}$) from the data, as the curve through the points cannot be represented by an equation²⁶. However, assuming an infinitely small concentration of salt results in the data point lining up with the linear fit on Fig. 8, the line can be extrapolated up to concentration 0.15 moldm^{-3} , giving 3.82g of solution absorbed, which translates into an absorption factor of 25.5 ± 9.00 . This corresponds to a percentage error of $\frac{30.0 - 25.5}{30.0} \times 100 = 15.0\%$ compared to the expected value of 30, the uncertainty encompassing the theoretical value.

²⁵ Uncertainties in this factor are composite and individual, as $factor = \frac{mass_{absorbed}}{mass_{crystals}}$, thus they

are calculated with the formula $\frac{\Delta factor}{factor} = \frac{\Delta mass_{crystals}}{mass_{crystals}} + \frac{\Delta mass_{absorbed}}{mass_{absorbed}}$.

²⁶ Attempts were unsuccessful in trying to give a linear or exponential equation to this curve.

Sample number	pH of sample	Absorption factor
2.1	3.00	8.40 (± 5.00)
2.2	4.00	9.73 (± 5.00)
2.3	5.00	8.00 (± 5.00)
2.4	6.00	11.40 (± 4.00)
2.5	7.00 (neutral)	30.30 (± 3.00)
2.6	8.00	29.50 (± 3.00)
2.7	9.00	32.40 (± 3.00)
2.8	10.00	31.50 (± 3.00)
2.9	11.00	32.00 (± 3.00)
Uncertainty	± 0.20	Individual

Table 4 Factor of their own weight that sodium polyacrylate crystals have absorbed with varying pH of solution

The absorption factor of solutions of pH 4.6 and 8.0 (the normal pH range of urine) can be calculated to be between 9.00 and at 29.5, respectively. It can then be noticed that the absorption of diapers widely depends on the pH of urine.

4. Explanation of results

The results obtained experimentally conform approximately to the models presented in the introduction. Since the results can consequently be interpreted as valid, it is necessary to analyze how they have come to occur.

For results involving change in concentration of sodium chloride in aqueous solution, it can be noticed that absorption decreases as sodium chloride concentration increases, linearly so by a factor of $-0.82 \text{ gmol}^{-1}\text{dm}^3$. The exception lies in the change in between concentrations 0.0mol dm^{-3} and 0.5mol dm^{-3} , where the decrease is much more pronounced. This is because when a solution with even a small amount of electrolyte in it (in this case sodium chloride) is in contact with sodium polyacrylate, the process of osmosis allowing the formation of hydrogen bonds with water molecules is immediately weakened by the presence of sodium cations in both reactants. Effectively, the polymer is no longer seeking to absorb as much water to balance the salt concentration inside and outside the polymer chain. Thus, the osmotic pressure that causes sodium polyacrylate to release its sodium cations bonded to oxygen decreases drastically. It can be said that the higher the concentration of sodium cations outside the hydrogel, the weaker the osmosis of water towards the gel, hence the weaker the absorption. This accounts for the linear relationship between the concentration of sodium chloride and the amount of solution absorbed, from the moment where some salt is present in the solution. Another explanation for this relationship lies in the fact that the sodium cations, in increasingly large number, whether it be the ones initially released by the polymer or the ones from the salt solution that have been attracted by the osmotic pressure, bond themselves to the anionic O^- sites on the polymer chain. The sodium cations thus prevent the water molecules from bonding to these sites, as the strong ionic bonding that the cations are seeking is stronger than the intermolecular hydrogen bonds that the water molecules are seeking. The neutralization of the ionic charges (between Na^+ and O^-) reduces the repulsion forces between the polyacrylate molecules in the polymer chain, caused by negative O^- valence charges, causing the chain to recoil. Thus, it collapses on itself due to its lack of polarity, losing its linear

configuration that renders it able to absorb water molecules. This collapse takes place even with small concentrations of sodium chloride, as marginal amounts of sodium cations within a solution are enough to significantly reduce the osmotic pressure that drives these ions towards the chain, significantly hindering the hydrogen bonding with water that would otherwise take place. This accounts for the change that does not conform to the overall linear trend, when looking at the curve's behavior between salt concentrations 0.0 and 0.5mol dm^{-3} . This theoretically immediate change supports the previous assumption that an infinitely small (yet not inexistent) concentration of salt results in a data point lining up with the linear fit for solutions where salt was added.

For results involving change in pH, it can be noticed that maximum absorption is situated in the alkaline pH range, and under pH 7.0 the absorption drops drastically and then decreases slowly, while over this value it is stable. When acid is added to the crystals, the Na^+ ions from the polymer diffuse by osmosis, allowing the uncoiling of the polymer chain, and the hydrogen cations from the acid, having reached the gel by osmosis, attach themselves through electrostatic attraction to the negative sites, once again preventing water molecules from attaching through weaker intermolecular hydrogen bonds. Consequently, absorption will decrease as pH lowers within the acid range (i.e. pK_a increases), as there are increasingly more hydrogen cations present in the solution, thus increasing the osmotic pressure driving them towards the gel, causing an increase in the number of ionic bonds between the O^- sites on the polyacrylate chain and these cations. This ultimately causes the polymer chain to collapse due to lack of polarity. Much like with the sodium cations in the previous experiment, an immediate effect due to an infinitely small amount of cations (this time hydrogen) within a solution could apply here as well, as the graph in Fig. 10 seems to suggest. It can be deduced that if acid is added to the gel instead of water, the solution, not possessing neutralized hydrogen and hydroxide ions in it, allows the carboxylate groups (R-COO^-) from the uncoiled sodium polyacrylate chain to become carboxyl groups (R-COOH), the monomers thus becoming carboxylic acids. When looking at solutions in the alkaline range of the pH scale, the hydrogel is subject to hydroxide anions from the base. Here, sodium cations once again diffuse by osmosis from the polyacrylate chain, resulting in its

uncoiling, and the presence of a base accounts for a minimal amount of hydrogen cations bonding to the polymer instead of water. The electrostatic repulsion between the carboxylate $R-COO^-$ groups and hydroxide (OH^-) ions does not in any way prevent the water molecules from their hydrogen bonding to the polyacrylate chain, which is why the variation for solutions of alkaline pH is virtually inexistent.

5. Evaluation

Even though the experiments approximately yielded the results expected, certain experimental weaknesses cannot be ignored, as they could have altered results. Due to the increased complexity of procedures, more weaknesses are to be accounted for in the experiment involving salt concentration than for the one involving pH.

Random error should not be overlooked, as the uncertainty of all measuring instruments was not negligible on the long run, as some solutions were transferred various times into different objects, and the uncertainties inherently cumulate. For instance, a sample of 2.5mol dm^{-3} sodium chloride solution came was made using a measuring cylinder with an uncertainty of $\pm 0.5\text{cm}^3$, whose content came from the large 3000cm^3 bottle with an uncertainty of $\pm 20\text{cm}^3$, whose own content came from two 2000cm^3 beakers both with an uncertainty of $\pm 10\text{cm}^3$, whose salt content was weighed on a balance of uncertainty $\pm 0.01\text{g}$. The monitoring of temperature (for both the room and the solution) was however carried out carefully.

Systematic error was rather more of a concern. The unreliability of the pH probe used, as various identical models' readings were slightly different for the same solutions, and readings often fluctuated indefinitely, could account for erroneous pH readings. To improve this, the use of more sophisticated probes (however not available in the school laboratory) could be considered. To otherwise overcome this weakness, the use of industrially prepared solutions (made from hydrochloric acid and sodium hydroxide) of appropriate pH could

have been considered, however they were not available in the school laboratory during the experimental phase.

For experiments involving salt concentration, the repeated transfers of the standard solution (from the big cylinders to the bottle to the small cylinders) meant that small salt deposits remained in every object after transfers. Moreover, small amounts of salt escaped the filter paper by osmosis during the gravimetric filtration to determine the standard solution's concentration. These two factors make the subsequent calculation of the concentration of the standard solution, and hence the concentration of all 100cm^3 samples, questionable. The use of suction filtration (using a Büchner funnel) to reduce error during filtration, or of a much more permeable filter paper, such as the Whatman Number 1 used for the pH experiment, could be considered. Also, when the reacted solutions were transferred into centrifuge tubes, marginal amounts of gel remained in the beakers and could not be entirely extracted, even by retransferring water in the beaker to wash the remaining gel out. This is one of the main weaknesses of the centrifugation technique. Another weakness of this technique was the deposition of very thin salt layers on the centrifuge tubes, once all the water had evaporated in the oven, leaving its salt content behind. The extra mass the deposits brought, even though very small (less than 0.10g), could have altered results. An alternative to the centrifuge technique, which consisted in using gravimetric filtration for each sample, was initially considered. It would have eliminated the error described above, but was abandoned because of the large amount of the time required compared to the centrifuge technique, and this time was simply not available. This technique was however used for the pH experiment, which includes fewer samples, and for which centrifugation would be too lengthy, as the amounts of solution absorbed are much larger, meaning the centrifuge machine would have to be used much more. The time constraints used up by these two lengthy experiments prevented full second trials to be made – although test trials had been done prior to each experiment – which would have added reliability to the results. The only incoherence in results was the calculated absorption factor of the 0.0mol dm^{-3} sodium chloride solution (distilled water), as the absorption factor was 68.6% off the 500-fold value expected. This could be due to the inefficiency of the sieve in retaining the

gel, in which case gravimetric filtration should be considered, or to impurities in the distilled water, not allowing it to absorb the predicted amount of solution.

As an evaluation of the sources used in this essay, it can be said that they were varied, coming from textbooks, internet articles (more and less academic), and scientific reviews. For internet articles, known as less reliable, validity was always questioned and attention given in order to double-check the reliability of the statements, by comparing two different websites on a given point. Only double-checked statements were used in the development of this essay's argument. The overall validity of textbooks and scientific reviews was considered less of a concern, thus these sources were not double-checked.

It can be said that despite various weaknesses in the experimental procedures, the results obtained have succeeded in confirming expected relationships, as they generally fit within the uncertainties established, enabling the interpretation of results as generally valid, and the drawing of conclusions directly from the data generated.

6. Conclusion

Having successfully investigated the influence of changing pH and changing sodium chloride concentration on the swelling of sodium polyacrylate, venturing through topics such as bonding, equilibrium, acids and bases, and organic chemistry, an answer to the research question can be provided. It can be stated that an increasing concentration of aqueous sodium chloride hinders the superabsorbent capacities of sodium polyacrylate, with respect to how it behaves in the presence of distilled water, and that there is a linear relationship between the salinity of a solution and the gel's absorption. As salt concentration increases, swelling effectively decreases. It can also be concluded that an acidic pH of a solution placed in contact with the gel yields very small amounts of solution absorbed, whereas the absorption rises sharply between pH 6.0 and 7.0 and remains high throughout the alkaline pH range.

However, this research on the properties of sodium polyacrylate is far from complete, and could be reinforced by further experimentation. For instance, the

sensitivity of sodium polyacrylate to other factors such as temperature and the strength of ions in solution could be investigated. A larger set of experimental data could contribute to making this study more precise, as salt concentrations of 0.25M, 0.75M, 1.25M... could be investigated, whilst ignoring the unyielding molarities over 3.0M. pH values of 3.5, 4.5, 5.5... could also be tested. An investigation on the kinetics of the swelling of sodium polyacrylate could also provide interesting material for a more complete investigation. The biochemical aspect of this research could be accentuated by testing sodium polyacrylate's absorption of different urine samples of known pH and salinity.

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9.1. Appendix I: List of apparatus

For production of standard sodium chloride solution:

- Sodium chloride powder
- Distilled water
- Weighing balance ($\pm 0.01\text{g}$)
- Temperature probe
- 2000cm^3 beaker (x2)
- Magnetic stirrer with flea
- Glass funnel
- Filter paper (x2)
- 3000cm^3 standard flask
- Oven

For preparation of different pH samples:

- 0.1mol dm^{-3} hydrochloric acid
- 0.1mol dm^{-3} sodium hydroxide
- Distilled water
- Temperature probe
- 100cm^3 measuring cylinder (x10)
- pH-meter with pH 4.00 and 10.00 buffer solutions

For preparation of samples of different sodium chloride concentration:

- 100cm^3 measuring cylinder (x13)
- Weighing balance ($\pm 0.01\text{g}$)
- Weighing boats (x13)

For sodium chloride and pH experiments:

- Dropping pipette
- Rubber corks
- Disposable HUGGIES Little Walkers Step-in nappy
- Scissors and scalpel

- Standard filter paper (for filtration of saturated sodium chloride solution)
- Whatman Number 1 filter paper (for pH sample filtrations)
- Sheet of paper
- 250cm³ beaker (x23)
- Stop clock
- Large glass funnels (x10)
- 500cm³ Erlenmeyer flasks (x10)
- Four glass centrifuge tubes (x12)
- Centrifuge machine
- Sieve (x2)
- Oven

9.2. Appendix II: Details: production of sodium chloride solutions

The theoretical concentration of a saturated solution of sodium chloride was calculated by taking a sodium chloride solubility curve, calculating the solubility at 23.5°C. This solubility was calculated to be 36.6% (or 366g/1000g). Since the molar mass of sodium chloride is 58.44g, the concentration of the solution is as follows:

$$\text{conc.} = \frac{n}{V}$$

$$n = \frac{366}{58.44} \approx 6.26 \text{ mol}$$

$$\Rightarrow \text{conc.} = \frac{6.26 \text{ mol}}{1000 \text{ cm}^3} = 6.26 \text{ mol dm}^3$$

It was assumed that sodium chloride has exactly the same density as water, as their densities are virtually identical. The table below shows quantitative data for the production of the standard saturated solution, done in two separate 2000cm³ beakers, with 1600cm³ and 1400cm³ of solution produced, for a total of 3000cm³. A known excess amount of salt was poured into both beakers, and after overnight magnetic stirring, the salt leftovers were filtered gravimetrically and put to dry overnight in an oven at 80°C.

Beaker	Mass of NaCl_(s) in water / g	Mass of filter paper + leftover NaCl_(s) / g	Mass of filter paper / g	Solution temperature / °C
1: 1600cm³	607.99	256.56	5.41	23.5
2: 1400cm³	542.57			
Uncertainty	±0.01	±0.01	±0.01	±0.1

Table 5 Quantitative data for production of saturated sodium chloride solution

Knowing the 256.56g excess of sodium chloride (including filter paper), the concentration of the saturated solution can be calculated:

$$mass_{total} = 607.99 + 542.57 = 1150.56g$$

$$mass_{undissolved} = mass_{undissolved + paper} - mass_{paper} = 256.56 - 5.41 = 251.15g$$

$$\Rightarrow mass_{dissolved} = mass_{total} - mass_{undissolved} = 1150.56 - 251.15 = 899.41g$$

$$\Rightarrow n_{NaCl} = \frac{m}{M} = \frac{899.41}{58.44} \approx 15.4mol$$

$$\Rightarrow conc. = \frac{n}{V} = \frac{15.4}{3.00} \approx 5.13mol dm^{-3}$$

$$\%error = \frac{theoretical - experimental}{theoretical} \times 100 = \frac{6.26 - 5.13}{6.26} \times 100 \approx 0.1805 \times 100 \approx 18.1\%$$

This large percentage error was then verified by dissolution of 36.60g of sodium chloride to form 100cm³ of solution, and stirred again overnight, to see if the errors correspond. The mass of the filter paper being 1.84g(±0.01), and the mass of the paper and the sodium chloride 11.84g(±0.01), the mass of non-dissolved sodium chloride was then 10.00g(±0.02). This implies that about 26.60g of sodium chloride had dissolved. Using the same calculations as above, this accounts for a percentage error of 27.3%, confirming the large error compared to expected values.

The following amounts of saturated solution to which dissolved water must be added in order to obtain 100cm³ of the solution of desired concentration were then calculated using the following example calculation.

$$amount_{saturated} = \frac{conc_{desired}}{conc_{saturated}} \times 100 = \frac{5.00}{5.13} \times 100 \approx 97.5cm^3$$

Concentration / moldm⁻³	Amount of saturated solution / cm³
Saturated 5.13	100
5.0	97.5
4.5	87.7
4.0	78.0
3.5	68.2
3.0	58.5
2.5	48.7
2.0	39.0
1.5	29.2
1.0	19.5
0.5	9.75
Distilled water 0.0	0.00
Uncertainty	±0.65

Table 6 Numerical data for dilution of saturated sodium chloride solution into samples of different concentration

9.3. Appendix III: Details: dilution of acids and bases

In order to obtain the desired pH values stated in the method, solutions of 0.1mol dm^{-3} hydrochloric acid and 0.1mol dm^{-3} sodium hydroxide were diluted serially. The pH of a solution of 0.1mol dm^{-3} hydrochloric acid is calculated:

$$-\log_{10}[H^+] = -\log_{10}[0.1] = 1 \quad \text{The pH of } 0.1\text{mol dm}^{-3} \text{ HCl}_{(\text{aq})} \text{ is } 1.00$$

By knowing that $pOH + pH = 14$, the pH of a solution of 0.1mol dm^{-3} sodium hydroxide can be calculated by calculating its pOH:

$$-\log_{10}[OH^-] = -\log_{10}[0.1] = 1 \quad \text{The pOH of } 0.1\text{mol dm}^{-3} \text{ NaOH}_{(\text{aq})} \text{ is } 1.00$$

Hence $pH = 14 - pOH = 14 - 1 = 13$ The pH of 0.1mol dm^{-3} $\text{NaOH}_{(\text{aq})}$ is 13.0

To obtain the different samples, serial dilution was used, by starting with solutions of 0.1mol dm^{-3} hydrochloric acid and 0.1mol dm^{-3} sodium hydroxide, whose pHs are calculated above. Because of the logarithmic relation between different pHs, it is known that by diluting 10cm^3 of the acid or base at concentration 0.1mol dm^{-3} with distilled water up to a volume of 100cm^3 , the pH will go from 1.0 to 2.0 for hydrochloric acid and from 13.0 to 12.0 for sodium hydroxide. 10cm^3 of both the acid and the base were then diluted up to 100cm^3 , each time with pH increasing by 1 or decreasing by 1, for acids or bases respectively. The solution with pH 7.0 was made from a neutralization reaction between hydrochloric acid and sodium hydroxide.