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Mathematical Modeling, Simulation and Prototype Designing of Potable Water System on Basis of Forward Osmosis

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Abstract **-** The development of Reverse osmosis happened in 1960. Along the years this technique has been widely accepted all over the world for varied applications ranging from seawater desalination to municipal water treatment. Forward osmosis (FO) is one of the foremost technologies for low energy consuming solutions for water purification. In this study we have carried out a detailed analysis on selection, design and pricing for a prototype of potable water system for purifying water in emergency situations. The portable and light purification system is envisaged to be driven by FO. This pouch will help serve as an emergency water filtration device. The current effort employs a model to understand the interplay of permeability and area on the rate of purification of water from any impure source / brackish water. The draw solution for the FO pouch is considered to be a combination of salt and sugar such that dilution of the same would result in an oral rehydration solution (ORS) which is a boon for dehydrated patients. However, the effort takes an extra step to actually estimate the cost and pricing of designing such a prototype.
While the mathematical model yields the best membrane (compositions taken from literature) combination in terms of permeability and area, the pricing takes into account the feasibility of such a solution to be made available as a retail item. The product is envisaged to be a market competitor for packaged drinking water and ORS combination (costing around $0.5 combined) and thus, to be feasible has to be priced around the same range with greater margins in order to have a better distribution. Thus, a proper business plan and production of the same has been formulated in order to be a feasible solution for unprecedented calamities and emergency situations.

Keywords**:** Forward Osmosis, Water Filtration, Draw Solution, Brackish Water.

1. Introduction

Water treatment is emerging as one of the most popular fields of engineering. Providing safe drinking water has become a challenge for various government agencies and municipal corporations across the world. While the nature of the problem remains same, the specifics related to treatment changes according to source and geographical locations. The present article is about a completely different aspect of water filtration where the possibility to filter brackish water has been addressed with help of a portable filtering pouch. The central idea is design of a forward osmosis (FO) driven pouch which will have a draw solution capable of filtering any turbid or brackish water so that the pouch gets filled with purified water and the solution ends up being an oral rehydration solution (ORS). Such technologies can help in being a great survival kit and for emergency situations like flood and rescue operations. Earlier authors have addressed such a solution through mathematical modeling. However, a detailed analysis including membrane types, physical properties like permeability as well as related economic analysis has not been addressed and is very important for possible prototype and product development leading to commercialization. The present article is about detailed investigation into a possible design of such a forward osmosis pouch. First, various FO membranes are selected from literature and the mathematical model is used to understand the effect of parameters, e.g., permeability and area of filtration, on the volume of water collected in the pouch. The target of the exercise was fastest collection of water using best combination of membrane and surface area of pouch. Second, the cost analysis and scale up analysis of such a pouch is investigated. The basic underlying principle being that the quickest fill up of the pouch using membranes and raw material costing of minimum value should be made possible so that a feasible retail price of the product. The benchmark price of such an item is compared with that of a combination of ORS packet ($0.33) and packaged drinking water ($0.33) which equals to almost $0.6. Importantly to the best of the authors' knowledge, this is the first report of a scale up analysis of such a product in order to make it a feasible substitute.

2. Determination of Osmolality

Different salts and sugars are taken for making three mixture solution which is commercially available in market[1].The osmolality vs dilution graph is plotted after performing experiments for each mixture solution[1].Then single graph is plotted for all three solutions using Power law.

Mixture one : (2M Sucrose + 0.1M Calcium Chloride)

The relationship between osmolality and dilution is expressed by power Law function. The best fit curve plotted from data points is shown by equation ($y=1.795x^{-1.0858}$) for mixture one[1].

Mixture two: (1M Sucrose + 1M Glucose + 0.1M Calcium Chloride)

The relationship between osmolality and dilution is expressed by power Law function. The best fit curve plotted from data points is shown by equation ($y=1.6298x^{-1.1177)}$ for mixture two[1].

Mixture three: "Dioralyte" Rehydration sachet

The relationship between osmolality and dilution is expressed by power Law function. The best fit curve plotted from data points is shown by equation ($y=2.467x^{-1.0292}$) for mixture three[1].

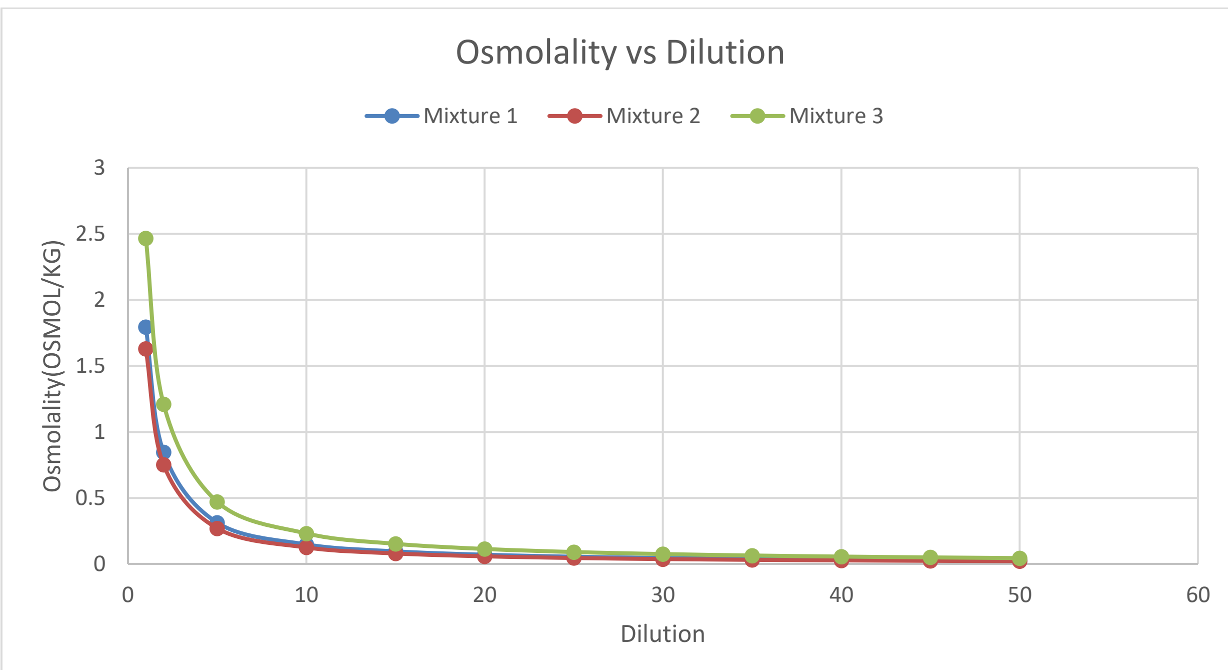

Fig. 1: Osmolality vs Dilution graph for all 3 mixture solutions.

2. Mathematical Modeling

2.1. Model Assumptions

The system is modeled in such a way that water of different concentration is separated by a membrane in (figure 4). The volume of water denoted by (1) is brackish water and volume (2) is potable water [1].

It can be assumed that the RO membrane is impermeable to all solute; therefore $j_s = 0$.The device will be used in large source of water; therefore $V_2 = \infty$ and Δp is only significant when the pouch is full [1].

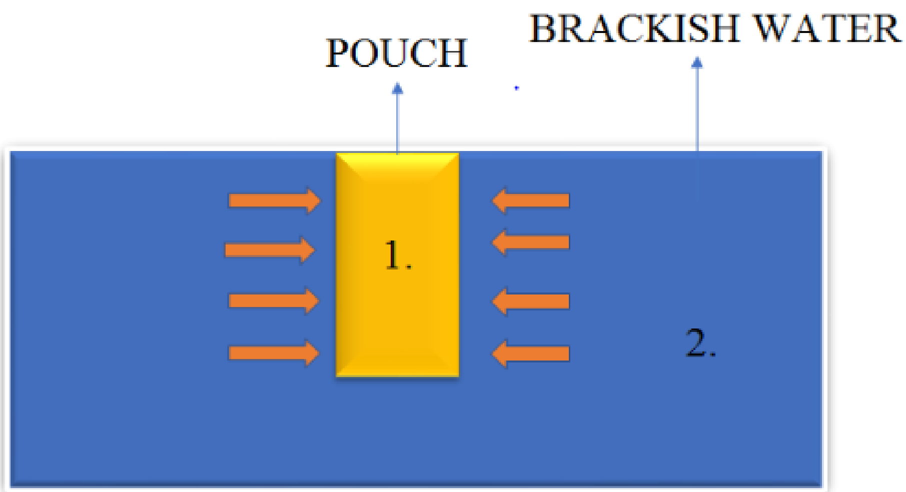

Fig. 2: Pouch is denoted by (1.) and brackish water is represented by (2.).

2.2. Modeling

The osmotic pressure can be defined as pressure acting to restore the chemical potential of a system [1]. Osmotic pressure (π) is denoted by the formula mentioned below:

$$\pi = c.R.T \tag{1}$$

Osmolality (M) is defined as solute osmotic concentration per mass of solvent. It is denoted by expression given below:

$$M = C.\phi.n \tag{2}$$

Now, substituting [Eq. (2)] in [Eq. (1)] gives an accurate prediction of the true osmotic pressure of solution in [Eq. (3.)]:

$$\Pi = M.R.T \tag{3}$$

The modeling of an 'RO' pouch is based on the principle that at low pressure no salt ions will be lost through the membrane. Therefore, a simple mass balance yields the membrane flux relationship.

$$J_V = L_P\,.(\Delta p - \Delta\pi) \tag{4}$$

Combining this result with equation (3), it can be shown that it is possible to obtain the result:

$$J_V = -L_P\,.R.T.(M_1 - M_2) \tag{5}$$

However, flux J_V can also be expressed as

$$J_V = \frac{dV_w}{A.dt} \tag{6}$$

Therefore,

$$dV_w = -L_P\,.R.A.T.\left(M_s^e - M_s^i\right).dt \quad (7)$$

Where

$$M_s^e = M_s^i\left(\frac{V_w^i}{V_w}\right) \quad (8)$$

i.e, a function of the dilution ,and $M = C.\phi.n$ as previously in Eq.(2).

2.3. Simulation

The simulation was based upon a pouch constructed of RO membranes having different hydraulic permeability taken from literature. For the simulation, mixture one is selected because it was able to fill pouch in minimal time[1]. In this simulation we are playing along only two variables i.e. Hydraulic permeability and area of membrane. The list of different RO membranes along with their hydraulic permeability is shown in table (1) as:

Table 1: Different RO membrane with different hydraulic permeability[2].

Membrane	Hydraulic permeability (LMH bar^{-1})
CAP-TFC (Cellulose Acetate Phthalate)	1.42
TFC with Lignin additive	1.88
SG-PAN (Polyacronitrile)	3.79
PAI-PES/PEI **(**Polyamide imide-polyethersulphone polyether Imide blend**)**	4.1
PAI/PES (Polyamide imide polyether sulphone blend)	15.9

Different variables and constants used for simulation is attached here in Table (2).

Table 2: Variable and constants used for simulation[1].

VARIABLES	
Surface Area of pouch (A), m^2	0.052
Initial external Molarity, (Osmols.kg H_2O-l)	0
Initial Pouch Volume, (Liters)	0.01
Time increment, dt, (seconds)	30
Final time for each sample, (minutes)	63 minutes
Initial internal Molarity, (Osmols.kg H_2O-l)	1.795
CONSTANTS	
Temperature, (K)	298.15
Universal gas constant I, (bar-L/mol-K)	0.08314

A Microsoft excel sheet was then set up using the expressions mentioned in 2.2 MODELING. The excel sheet calculates the dilution within the pouch as a function of time with an interval of 30 sec $(= t + dt)$ and uses this value to determine the molality within the pouch from power law. Expression is then used to calculate the change in volume over that time increment, which is added to a running total volume[1]. Individual excel sheets were made for all five membranes and volume of water collected at the end of 63 minutes is shown in single graph (figure 5) for all membranes. The data extracted from above excel sheets for all five membranes is further used for plotting the graph of volume vs time. All curves of five membranes are then shown in figure 3

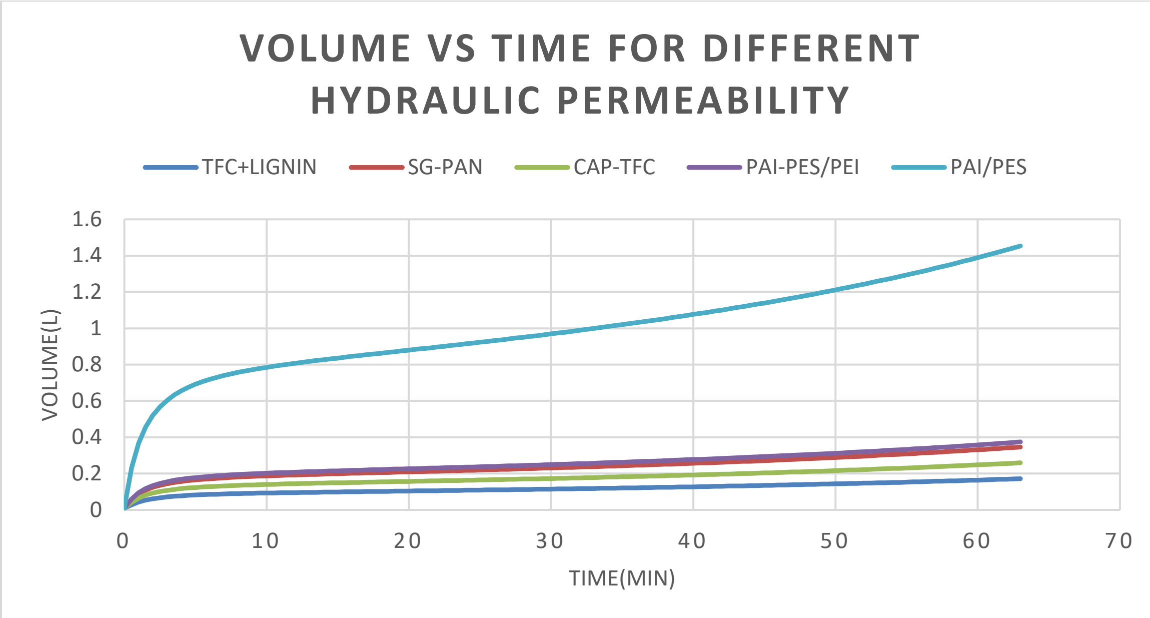

Fig. 3: Volume of water collected inside pouch made up of different membranes at the end of 63 minutes.

2.4. Area Analysis

From previous permeability and sensitivity analysis two best membranes are selected. Now, for a particular membrane keeping all parameters constant, area of pouch is varied in such a way that it is increased by 10% from base area (0.052 m^2) in each interval and their effect on collection of volume of water at the end of 63 minutes is done in excel sheet. Membranes selected are PAI-PES/PEI and PAI-PES, whose area is increased from 10%(minimum) to 50%(maximum) from its base area (0.052 m^2). There are total five curves in increasing order denoted by symbols A1(10% increment in area), A2(20% increment in area), A3(30% increment in area), A4(40% increment in area), A5(50% increment area) shown in figure 4 and figure 5.

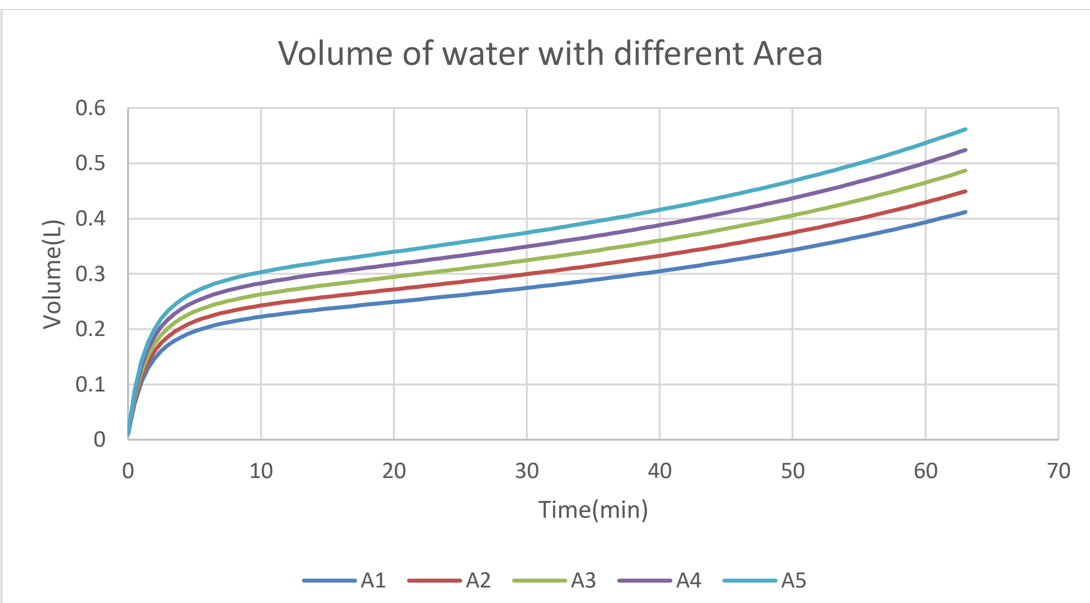

Fig. 4: Volume of water collected at the end of 63 minutes by pouch of varying area in increasing order(A1<A2<A3<A4<A5) for PAI-PES/PEI.

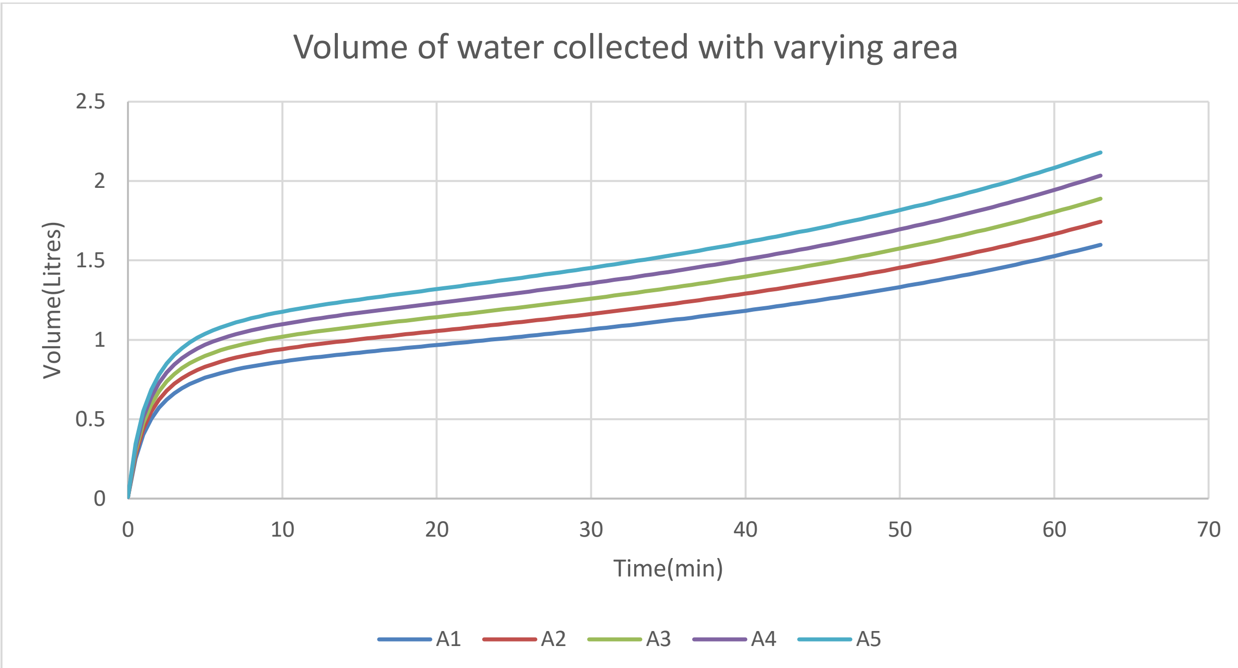

Fig. 5: Volume of water collected at the end of 63 minutes by pouch of varying area in increasing order(A1<A2<A3<A4<A5) for PAI/PES.

3. Cost Analysis

A case of flood in South India during 2015 is studied and taken as basis for cost analysis. There were total 1.8 million people affected[2]. According to WHO standards the daily water requirement by adult for drinking is 2 Liters. Total water requirement for drinking water was around 3.6 million Liters per day. The pouch which is proposed here is capable of collecting total 500ml of water. Total pouch requirement on daily basis was around 15 million. The pouch also contains ORS which acts as draw solution. The benefit of using pouch is that it will keep people rehydrated in such catastrophic scenario. The area of pouch is taken as equivalent to two A4 size sheet which leads to total pouch area of 0.12474m^2 . The spacing between pouch is 0. 03m.The volume of pouch is around 1 Liter. The costing is done on the basis of wholesale price of Indian market. For pricing of raw materials mentioned in (Table 5 and Table 6) various distributing companies are contacted and their approximate price is investigated by them. The material requirement, its quantity and price for designing a single pouch is mentioned in table:

Table 3: Materials requirement and their quantity for making pouch of area 0.12474m^2 .

Polymer Requirement	16 grams
Solvent	84 grams
Draw Solution	100 milliliters
Miscellaneous	Membrane support, Plastic pouch and accessories

The best membrane was chosen from the above analysis i.e. Polyamide-imide and Polyethersulphone blend(PAI/PES). The cost analysis is done further for this membrane.

3.1. PAI/PES (Polyamide-Imide and Polyethersulphone Blend)

The best composition for maximum water flux for PAI /PES blend membrane is having weight percent of PAI as 40% and weight percent of PES as 60% [4]. Synthesis of PAI is done by polycondensation of Diimide-Diacid(DIDA) and p-Phenylenediamine(PPDA)[5].

3.1.1. Materials

Synthesis of PAI

- Diamine
- Diimide-diacid(DIDA)
- Triphenyl phosphite
- N-methyl-2-pyrrolidone (NMP)
- Pyridine
- Calcium chloride

Synthesis of PAI/PES Blend

- Dimethylacetamide (DMAC)
- Polyethersulfone (PES)
- Polyvinylpirrolidone (PVP)
- Polyamide-imide(PAI)
- 2-Propanol (IPA)
- Distilled water

For the synthesis of blend of PAI/PES, first of all basis of 100 grams of polymer and solvent is taken for synthesizing membrane of area 0.12474m^2 [6]. Then further cost analysis is done for 15 million pouches.

Synthesis of PAI/PES blend require following materials in given quantity [4].

- PAI/PES=16g
- PAI (40%)=0.4*16=6.4g
- PES= (60%)= 0.6*16=9.6g
- PVP= 2 g
- DMAC=82 g

Before the synthesis of blend, first of all PAI should be synthesized. So, the basis taken for synthesis of 1 gram of polyamide is mentioned in Table 4.

Table 4: Quantity of materials for synthesis of 1gram Polyamide-Imide(PAI)[5].

Materials	**Quantity**
Diimide-Diacid, gram(g)	0.790
4,4 – Methylenedianiline, grams(g)	0.248
Calcium chloride, gram(g)	0.8
NMP, milliliter(ml)	8
Pyridine, milliliter(ml)	1.5
Triphenyl phospite , milliliter(ml)	0.8

For synthesis of 1 pouch, 6.4g of PAI is required then for 15 million pouches the requirement of materials for synthesizing PAI is mentioned in table:

Table 5: Quantity of overall materials required for synthesizing PAI which is further used in synthesizing for pouches.

Material	**Quantity**	**Price ($) US Dollar**
Diimide-Diacid, kilogram(kg)	75840	$8.5*10^4$
4,4 – Methylenedianiline, kilograms(kg)	23808	$2.21*10^4$
Calcium chloride, kilogram(kg)	76800	$9.5*10^3$
NMP, Kiloliter(kl)	768	$1.1*10^6$
Pyridine, Kiloliter(kl)	144	$1.1*10^5$
Triphenyl phospite , Kiloliter(kl)	76.8	$9*10^4$

Total cost of synthesizing PAI is $ $1.46*10^6$ [Table 5]. For synthesis of 15 million pouches the requirement of materials is mentioned below:

Table 6: Quantity and price of materials required for synthesizing of 15 million pouches.

Material	**Quantity(KG)**	**Price ($) US dollars**
Polyamide-imide(PAI), kilogram(kg)	$9.6*10^4$	$1.46*10^6$
Polyethersulphone(PES), kilogram(kg)	$1.44*10^5$	$1.35*10^5$
Polyvinylpirrolidone(PVP), kilogram(kg)	$3*10^4$	$7*10^4$
Dimethyl-acetamide(DMAC), kilogram(kg)	$1.23*10^6$	$7.65*10^5$

Manufacturing cost is summation of production, labor and capital cost.
Thus, the manufacturing cost of 15 million pouches are = $ 2.4 Million
Manufacturing cost of single pouch is around =$ 0.15
Cost of ORS-solution for 100 ml = $ 0.15
Hence, total cost of portable device (draw solution +membrane-based pouch) = $ 0.3

4. Remarks on Cost Analysis

According to the simulation of the best membrane which can be synthesized, the portable device can fill 500-600 milliliters of water in 8- 10 minutes with given area of membrane i.e. 0.12474 m^2 and considering the efficiency of pouch to be around 60-70%. This water has ORS solution also which adds an extra benefit to health. This device can be used by army, flood victims,athletes, trekking people etc. This is lighter in weight so flood relief team can carry more pouches than regular bottles and price is also optimized around $0.23. Solvent can be used again in synthesis of pouch that's why price come down $0.23 to from $0.30. This product can be distributed in market including profit at around ($ 0.5).

5. Experimentation

After simulation and cost analysis, experimentation is carried out for checking the feasibility of concept of forward osmosis pouch. The membrane and draw solution taken for this experiment is Polyamide membrane and commercially available Iodised salt.

Polyamide membrane pouches are taken with different exposed area. The hydraulic permeability of membrane is 12 LMH bar^{-1} . A draw solution is prepared by taking 200ml of normal drinking water and commercially available Iodised salt. The solution is made supersaturated at the room temperature of 298.15 K. It is kept for 60 minutes in turbid water as can be seen in Fig 7.The results are observed for the same and shown in the Table 7.

Table 7: Amount of water collected from turbid water source inside pouch after 60 minutes.

Serial number	Exposed Area, m^2	Volume of draw solution(ml), V_1	Total Volume of solution (ml), V_2	Net water movement inside pouch(ml), $V_{net} = V_2 - V_1$
Pouch 1	0.0108	26	58	32
Pouch 2	0.0216	50	83	33

The experiment has been conducted in the lab and pictures and their description is also added in this paper in appropriate sequence.

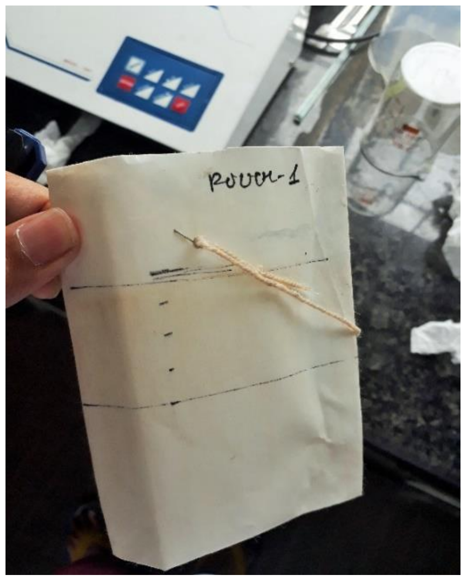

Fig. 6: Polyamide membrane pouch.

Fig. 7: Pouch kept in turbid water.

Fig. 8: Initial water level of beaker.

Fig. 9: Decrement of water level in beaker after 60 minutes.

The picture shown in Fig 9 shows the decrease in level of water in beaker because the water has moved inside the pouch.

7. Conclusion

After carrying out the experiment, we can conclude that the forward osmosis pouch is capable enough of collecting potable water from the turbid water source without any impurity in 60 minutes. This simulation demonstrates that the forward osmosis pouch can be used as emergency drinking water system. Currently we are working in our lab on optimizing the area, permeability, costing and choice of draw solution to make the most efficient membrane in coming future.

8. Symbols

A - *Pouch surface area, m*^{2}
c - Concentration, mol/m^3
J_V - Water flux,
j_s - Solute flux
L_P - Hydraulic conductivity
R - Universal gas constant
T - Temperature, K
M_s - Osmolality of solution, Osmoles-kg^{-1}
t - time
V_w - Pouch water volume, m3
n - Dissociation number
p - Hydrostatic pressure, Pa
Greek
Φ - Osmotic coefficient
Π - Osmotic pressure, Pa
Superscripts
e - External
i - Internal

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