AGENT BASED MODELLING FOR CAPILLARY ACTION SYSTEM PHENOMENA

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ABSTRACT

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1 INTRODUCTION

The study of liquid mechanics, in particular water, has been very important over the development of science and the construction of civilization and mankind as we know it. The study of fluid mechanics allows us to develop better tools, machinery and processes, or at least use science to prevent liquids to harm the improvements in our lives and also, how scientist with their studies have learnt to use the properties of fluids in our favor. For example with hydraulic presses, dams to generate power, and even huge irrigation systems to our crops. With these ideas in mind, water and fluids in general are very relevant in our daily life, in particular, water, important to even our own existence. Thus, the main purpose of this work is to model how fluids behave under certain circumstances, as in the capillarity phenomenon. A process that also occurs in one of the most marvelous and important processes, photosynthesis.Capillarity is also important for the well functioning of the pipelines and aqueducts systems. This phenomenon is also responsible of the transport of nutrients in our body. In summary, capillarity allows to transport fluids, in particular water, efficiently and easily, as it is natural process. The main objective in this work is to model this physical phenomenon using an Agent Based Modeling, as the agents represent molecules of a fluid.

2 CONCEPTUAL MODELLING

To design the conceptual model the ODD protocol (Railsback and Grimm 2019) was the perfect tool to develop it.

2.1 Overview

2.1.1 Purpose

The system to model represents the capillary action phenomenon, in which a liquid (for example water) thanks to surface tension, its cohesion and other physical and chemical properties is able to ”climb” a tube, or the space in which is contained. For example, we see this process in plants in their xilem and phloem during the photosynthesis.The importance of this model is its great applicability, as liquids mechanics are important to material sciences, biomedical studies and industrial engineering in general.

2.1.2 Entities, state variables, and scales

The principal agents in this model are the water particles, or liquid particles in general. Characterized by density, diameter, circular shape and color. These particles are in a ”U” shape container with a tube or capillar in the middle, essential to the capillary action phenomenon to take place. The molecules interact with each other, as they causes attraction forces due to Newton's Law and the Nuclear Force, besides gravity is also applied to them. The time scale is for some minutes, as this process is almost immediately, represented by minutes and sometimes even seconds.

2.1.3 Process overview and scheduling

The particles are grouping up, as they are attracted to each other (cohesion) and as they get closer to the tube they start to "climb" it, as the capillary action phenomenon says. Also, the particles are affected by other forces, like gravity. The schedule of the model first the particles are set up randomly, but inside the "U" shaped recipient. Soon after, as they are close to each other, they start to group up, forming bigger molecules. Also, the molecules move up along the forming tubes as long as the cohesion forces are stronger and the capillary action phenomenon takes place.

2.2 Design concepts

- **Basic principles**
  The model is an agent based approach to the capillary action of some liquid elements. In particular, water, and how its particles interact with each other. The theories that are underlined by this approach are: Jurins Law, Liquid transport and Surface tension.
- **Emergence**
  The model must show how the nearest particles to the tube are climbing it, just as the capillarity action describes. This as a consequence of the movements that the particles described, based on Liquid transport theory.
- **Adaptation**
  The agents can respond depending of the width of the tube. If it meets the conditions to climb it, they will, if not, they wont. The agents follow an indirect objective-seeking as they follow patterns well observed in science and real life systems.
- **Objectives**
  As all agents must follow a pattern, only those that interact with the tube are of interest. As these are the ones that will climb and do the capillarity action
- **Learning**
  The agents doesnt learn, as they represent molecules of a liquid, in particular, water particles that follow a chemical process.
- **Prediction**
  The prediction process is not prediction at all, is implied in the adaptative traits of every single agent. This determined by their behaviour when they are close to the tube.
- **Sensing**
  Every agent interacts with each other. As they represent water molecules, attraction and repel forces are always acting over them.So every agent must sense their surroundings, to know which particles are the nearest and attract or repel to them.
- **Interaction**
  As discussed in the previous item. Every agent interacts with each other. As they represent water molecules, attraction and repel forces are always acting over them. Groups can be formed, if they are too close. And being together like this causes the capillarity phenomenon. The distance to calculate vicinity is very small, as they are particles and are, generally, very close to each other. However, repel forces are also taken into account, in order to fulfill Paulis principle.
- **Stochasticity**
  As this model describes a well known physical model, the capillary action, a deterministic phe-

nomenon, the process is not stochastic per se. However, the initial position of the water molecules is set randomly.

- **Collectives**
  Collectives are not really taken into account. However, clusters of particles may form, but their behaviour is the same of just one agent. As they represent the same physical process.
- **Observation**
  In order to realize if the model is correct or no, a visualization of the water climbing is enough, as it is fulfilling the purpose of represent capillarity. However, validation must be done, checking with physical and chemical formulations related to the phenomenon.

2.3 Details

2.3.1 Initialization

The model starts with 1000 particles of water, their position is set randomly, but inside the ”U” shaped recipient. Other initial consideration is the acceleration of gravity, being an study done here, the value is $9.8m/s^2$. Also the wide of the tube can be set manually. The density of the particles is also a parameter, so an slide allows the user to change its value, in order to decide what kind of liquid particles are interacting.

2.3.2 Input Data

The data for the model is given by parameters, such as density, diameter of the particles, the force of attraction between particles. Also the repel force between them. Finally the width of the capillar that the liquid will ”climb”.

2.3.3 Submodels

The randomize submodel sets the x and y coordinates of the particles randomly. As long as they are inside the recipient.To do the this a create walls submodel is also used. This sets the box/world borders as they were real borders of a glass recipient. And to set then randomly, the randomize command checks if the coordinates are inside or not the bounded space. Then interact-with-neighbor comes to action, the particles come closer to their nearest neighbors.The parameter water-force is related to this submodel, as it determines with how much force the particles attract to each other. Also repel-too-close, prevent that the particles are one over the other, in other words, following Paulis principles in a particles is in a determined place in the space no other particle can occupy that place. To bounce allows the particles to change direction if the crash to a wall of the recipient, this is bouncing in the wall.This is done asking whether the next patch (the one ahead in its direction/heading) is green, as this is the color of the recipient.

3 BACKGROUND

Biological phenomenons and processes are thought to be entirely deterministic, but actually both influences, between stochasticity and determinism, has shown more accurate results. ”These findings support the use of rule-based approaches for modeling the complex mechanisms underlying sprouting angiogenesis over purely stochastic methods.” (Walpole, Chappell, Cluceru, Mac Gabhann, Bautch, and Peirce 2015) . Where angiogenesis was simulated to evaluate endothelial cell sprout and the ABM approach, with both deterministic and stochastic characteristics, was more accurate than just a Monte Carlo model. Thus, the literature shows that stochasticity must be taken into account in order to add realistic features to the model. Other approach related with this work is the Raindrops model (Wilensky 1998) where the surface tension is an important parameter in order to model accurately enough the movement of other water particles after they are affected by an external force (in this example, the fall of raindrops and the waves it causes) a biological and chemical phenomenon that is very related with capillary action.The importance of Agent-Based Modelling for capillarity action is wide. Since applications in biomedical studies and science to microfluidic devices to control reactions. Besides, systems with these characteristics (ABMS ones) offer low cost alternatives to experimentation (Smith and Gaver III 2010). As the efficacy of these designs depends of the mechanics of the fluid the importance of Agent Based Modelling approach is more noticeable, as ABMS offers accurate and efficient simulation techniques.

4 MODEL INPUTS

The model represents a real life phenomenon, capillary action. In this process the main actors are the liquid particles in the recipient and a tube, as this is the element that the liquid will climb. Obviously, the forces that affect all these elements must be taken into account, so laws of physics are involved. First of all, to determine the size of every particle, the density of it must be take into consideration. To do this the dimensions of the world are also important parameters, this because the size of the agents cant be too big. So to settle this the equation that allows the particles to have a good size is $\sqrt{(rho * l * h)/n}$, And this expression sets the diameter for every particle. Where:

- ρ : the density of the particle
- l : the world-width
- h : the world-height
- n : the number of particles

Other important factor is the width of the tube, since this is one of main factors for the capillarity to occur. To set the tube, the user can choose the width of it, also the coordinates of py-cor, px-cor and min-pycor are taken into consideration. Since it must be in the center of the box, to produce a more homogeneous result. Other important action is the interaction with the other particles. The command interact with neighbor represents the attraction forces that every molecule is affected by. Checking the distances with the others, if the near particles are within the radius of interaction, the will attract each other, besides the direction they are facing changes, according to their nearest neighbor (nearest molecule). When introducing gravity force affecting the molecules, Newtons Law explains the behavior $h = v_0 t + \frac{1}{2} g t^2$, and this describes the position. As the initial speed v_0 is zero, this disappears of the formulation. And the position of the particles doesnt change much, as the particles below hold the ones above. Other important consideration is bouncing, as the particles do this in real life. However, this didnt need a hard mathematical formulation. If the patch ahead was green, the color of the recipient, the direction of movement changed, as if the particle had collided with it. Also, collide between particles were modeled. The vectorial components of a particle position, $\cos(\theta)$ and $\sin(\theta)$ and the corresponding geometrical interaction between them, changing its heading, depending of the current position and the angle of the collision. Finally, the forces between the water particles and the tube. This is one of the most important components of the model, as it represents the force that allows the particles climb the tube. Jurins law allows explains this behavior. $h = \frac{2T}{\rho r g}$ where the height achieved by the liquid is defined by this expression

5 IMPLEMENTATION

In order to develop the model, the software selected is NetLogo Version 6.1.1. (Wilensky 1999) Where the blue dots represents particles of a certain liquid, in general water. The red patches, the tube, necessary for the phenomenon to happen. The initial setup of the model looks like the following image.

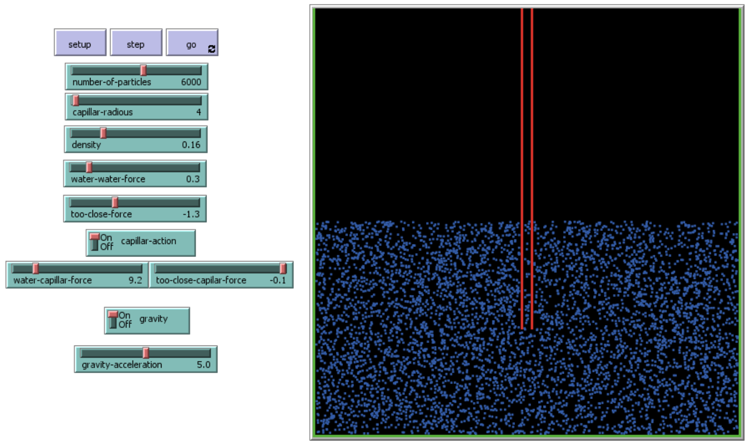

Figure 1: Initial data

Where the sliders in the left allow the user to change certain parameters needed to the phenomenon to occur, or at least do it under certain special considerations.

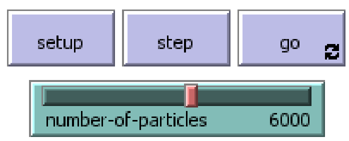

Figure 2: Setup buttons

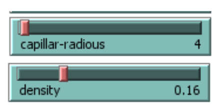

Figure 3: Capillar radious and density

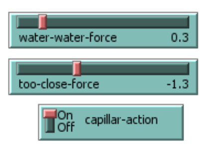

Figure 4: Water force, capillar action and too close force

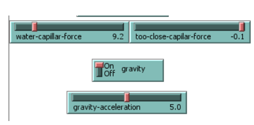

Figure 5: Combination of forces that change the behavior.Between water and the tube, gravity and the repel force

This set of sliders and parameters allow the interactions between the particles, and whether they climb the tube or not. Good parameters, like low density and high force for interaction between the particles allow an easy to catch the capillarity phenomenon along the appearance of a meniscus.

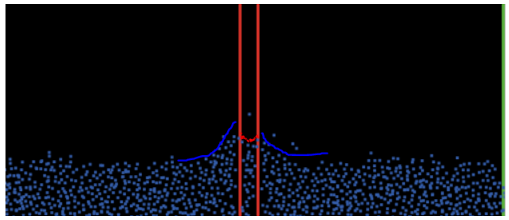

Figure 6: Meniscus formation

Other consideration that must be taken into account is the set of good parameters, that will be discussed in the next items, because impossible physical sets will lead to impossible results, however they are left in order to the user and experiment how living in other planet, or changing the laws of physics could affect the way the fluid behave. Finally, the running time should be low, as one tick passes when all the agents move or interact at least once. With this in mind, as there 6000 agents (in the setup configuration) time passes only when they all interact (as they interact all at the same time)

6 VALIDATION AND VERIFICATION

In order to validate the model, we are able to evaluate in there, the capillary action described by the equation given the Jurin's law.

$$h = \frac{2\gamma}{\rho r g} cos\theta$$

where γ is the surface tension measure, θ is the angle of the resulting triangle between the ratio of the meniscus for its spherical hood and the ratio of the capillar . But, in this case, this model is lack of many real measures like the surface tension, the viscosity, or the good implementation of the gravity or the atmospheric pressure. This make difficult the way of validate the system with the real equation of the phenomenon. It's important to know that, the system itself is modelling so many procedures of liquids, like collisions between particles, cohesion and repulsion forces and adhesive forces. So that, the only way to validate the model without a numerical analysis is in a empirical way, where it is possible to see that with the right parameters , the system itself reflect the right behaviour like:

- Meniscus in the capillar and in the right and left side of it
- The particles, in a general therm, are stables because of the gravity, collisions, cohesion and repulsion forces

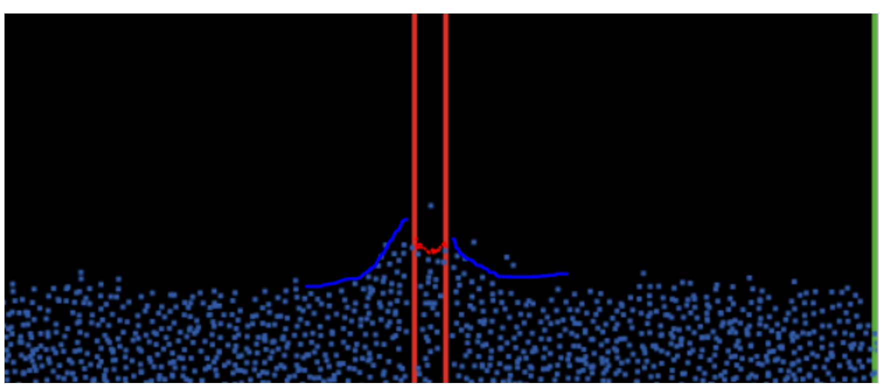

Figure 7: Meniscus formation

The particles by themselves have a good and stable behaviour in the time-step of the model. The parameters which show good results are:

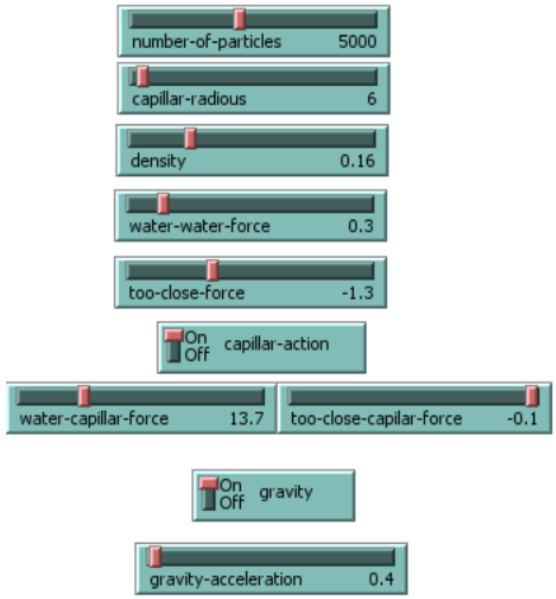

Figure 8: Stable parameters

7 EXPERIMENTATION

First of all, it is possible to run the model without gravity. In that way the bottom of the capillar is not able to fill the particles which the capillar takes at the first instance. So that, if in the beginning it starts winning, the final behaviour tend to take away the particles in the bottom of the capillar.

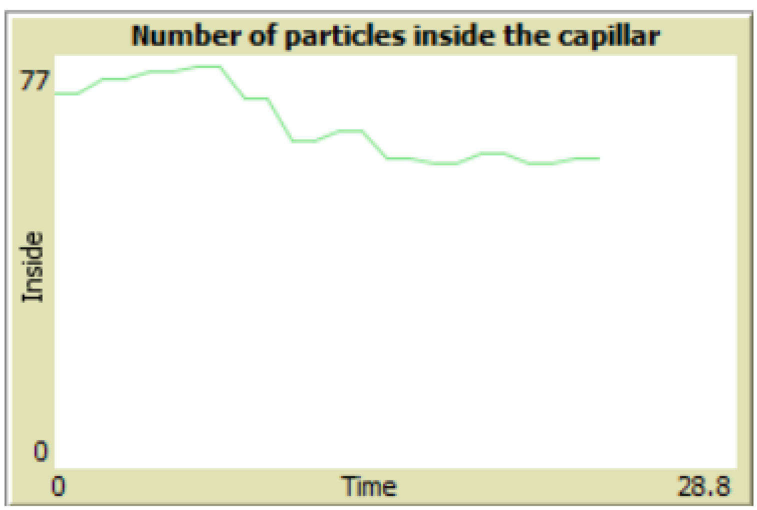

Figure 9: Number of particles inside the capillar.

If the gravity takes high values. the model tend to collapse, because it can not keep ahead high levels of that variation.

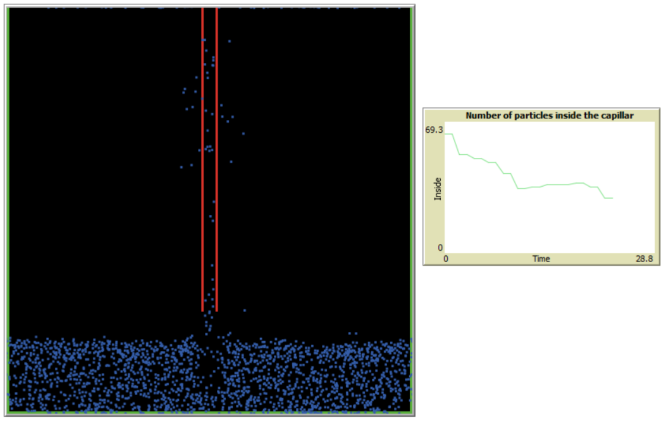

Figure 10: Effects of high values of gravity

If parameters like water-water-force are so high, which refers to the measure of the cohesion force, the liquid evidently tend to group itself in closer groups, thing that make the capillary action a harden phenomenon. If the water groups up, the capillar will be not able to take it.

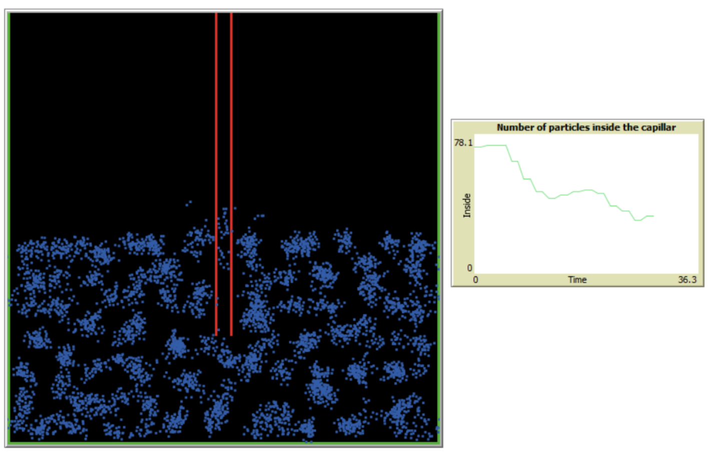

Figure 11: High level of cohesion force

The parameter which refers to the adhesion force is the water-capillar-force. If this one get higher than 15, the system tends to destabilize as it is showed in the next figure:

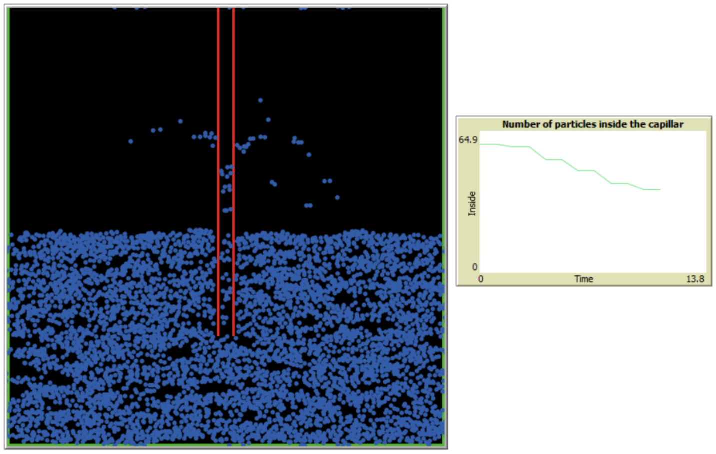

Figure 12: High capillar force effects

Finally, the too-close-force itself is the less sensible parameter. This happen just because of the collisions of every particle with the others, that is why this parameter is not so needy in every turtle action, however, it is necessary to express the repulsion force between particles.

8 CONCLUSION AND ADVICES

The model shows a good approach to the capillarity phenomenon. As the meniscus appears given a correct set of parameters specifications. Fulfilling the objective to model the capillarity action using an Agent Based Modelling Approach. However, the phenomenon is far to be completed, as many other variables can be measured and they also affect the behaviour of molecules.For example, temperature affects water, as it boils it, so the particles behave differently under this circumstance.To measure the performance of the model, just counting the number of particles and how they behave inside the capillar should not be the only way of measurement.Other physical laws like the Jurins one, that determines the height achieved in the capillarity phenomenon should be used. For future work, the model should use more variables and physical characteristics to extend the analysis that can be done.

Regardless, the model it is not just good a modelling the effect of capillary action. It is also good at modelling the interactions between liquid molecules which are suppressed to cohesion, repulsion and gravity forces.

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