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Simulation of Heat Diffusion Phenomenon by Using Netlogo and Comsol Multiphysics

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Abstract
Heat diffusion is the rate of temperature spread through a material. It is the measurement of heat transfer of material from the hot to the cold end. A two-dimensional plate of rectangular shape was modelled by using Netlogo and COMSOL Multiphysics. Netlogo is the agent-based modelling (ABM) simulation software that used to measure and investigate the movement of particle heat diffusion. While COMSOL Multiphysics that based on finite element method (FEM) was used to structure the model of rectangular shape and to solve the heat diffusion equation with the boundary conditions. This study is to investigate the simulation of heat diffusion phenomenon using two different approaches using Netlogo and COMSOL Multiphysics through the two-dimensional plate of rectangular shape model with different times, temperature and boundary conditions. The simulation results show that the two different approaches of heat diffusion are highly satisfactory based on their time and temperature in different position of two-dimensional plate of rectangular shape.
Keywords: Heat diffusion, ABM, Netlogo, COMSOL Multiphysics

1. Introduction
The true origins of any method or procedureare seldom identifiable in an unambiguous manner. In the case of agent-based modelling, one could think of Craig Reynolds' 1987 seminal article on the formation of Agent Based Modelling of Bird flocks(with the agents denoted as *boids*, short for "bird-oid object"), which he was able to represent with just three rules of behavior: (1) avoid collisions with nearby birds; (2) attempt to match the velocity of nearby birds; and (3) attempt to stay closeto nearby birds in the flock (Reynolds 1987; Gooding 2019). The result of simulations with this simple ABM was very realistic-looking flocking behavior. Particularly intriguing in this study was the fact that there was no leader or a global organizing principle. Instead, the virtual birds were truly individual agents that self-organized locally, thereby generating a globally coherent flight pattern.

While Reynolds' work was a milestone, key concepts leading to modern ABMs can be found much earlier. One notable contributor of ideas was Nobel laureate Enrico Fermi, who used mechanical addition machines to generate probabilities for stochastic models with which he solved otherwise unwieldy problems (Gooding 2019). This procedure was an early form of the method of a Monte Carlo simulation, which waslater independently developed and published by Stanislav Ulam, like Fermi a member of the Manhattan Project (Metropolis & Ulam 1949; Metropolis 1987). Another very important contribution to the budding development of ABMs was the Turing machine (Turing 1936), which is a mathematical model of computation that uses a set of rules to manipulate symbols in discrete cells on an infinite tape. Much closer to ABMs were ideas of Ulam, who was fascinated by the "automatic" emergence of patterns in two-dimensional games with very simple rules (Ulam 1950; Metropolis 1987).

Next, the software that had been used in agent-based modelling, since the research title is based on concept of agent-based modelling, is Netlogo. NetLogo (Wilensky, 1999) is a modeling environment designed for coding and running agent-based simulations.[1] Nowadays, there are many languages and software platforms that can be employed to create agent-based models,[2] and at the time of writing NetLogo is the most widely used. We recommend NetLogo and will use it throughout this book for the many reasons we outline below. The language used to code models within NetLogo –which is also called NetLogo– has been designed following a good philosophy (Wilensky and Rand, 2015). All reviews of the software highlight how easy it is to learn. To be concrete, we would estimate that an average scholar without previous coding experience can learn the basics of the language and be in a position to write a simple agent-based model after 2-4 days of work. Someone with programming experience could reduce the estimated time to 1-2 days.

One characteristic that makes the NetLogo language easy to learn is that it is remarkably close to natural language. As a matter of fact, NetLogo language could perfectly be used as pseudo-code to communicate algorithms implemented in other languages.

On this topic, there also have a numerical simulation software that be used which is COMSOL Multiphysics. While transport phenomena textbooks are good at presenting the fundamentals, most of the problems are one-dimensional, since that is the limit of the mathematical ability of most undergraduates. Today's students are motivated by real-life examples, but they have limited time. With the advent of sophisticated software, however, it is possible for undergraduates to solve meaningful transport and flow problems in two and three dimensions. This talk presents the methods used to introduce undergraduates to COMSOL Multiphysics and the problems they solve in a research project format. The learning occurs in three stages. First, the students learn to solve problems in their textbooks and learn to validate the solution. This gives confidence that the computer program is solving the right equations. Next, they solve more complicated 2D problems, which go beyond their textbooks by removing assumptions. In this stage, students are confronted with the necessity of translating their problem into the notation of the computer program and proving they have solved the problem correctly even though there is no analytic solution. They learn how to check their data input to the program, look for artifacts in the solution, and use mesh refinement to estimate the numerical error. They explore the many ways to analyse and view the results, from streamlines, contour plots, integrals, etc. of the dependent variables as well as derived quantities (defined in terms of the dependent variables). For example, is the total flow in equal to the total flow out? – not a straightforward question when there are multiple inputs and outputs and the solution is numerical. The second step is illustrated in detail to show the breadth of analysis techniques. The third stage in the learning process is to solve their research problem. Valuable features of COMSOL Multiphysics include the graphical user interface, the tools for creating the geometry and internal boundaries and domains, automatic mesh generation and refinement, the ability to solve different equations on different meshes (all in the same problem), the multi-physics capability which permits addition of equations to represent additional phenomena, the ability easily to make parameters depend upon the solution, the parametric solver, and the post-processing graphical features (Finlayson, 2006).

Some of calculation need to use a method that been studied on part in numerical method.

2. Literature Review

2.1. Simulation of Heat Diffusion Phenomenon

In this study, 3D heat diffusion by conduction in the proximity of a 3D defect is modelled using a boundary element method (BEM) formulated in the frequency domain. The defect is a crack lodged in an unbounded solid medium with null thickness. In order to overcome difficulties that occur in the presence of null thickness elements, the BEM formulation was written in terms of normal-derivative integral equations (TBEM) and known analytical solutions were used to solve the resulting hypersingular integrals. The focus of this paper is to study the influence using either a 3D (point) energy source or a 1D (planar) energy source in heat diffusion simulations performed for IRT defect detection studies. Heat field and thermal wave phase results were computed in the presence of a defect and for when there is no defect present and a comparative analysis of the results obtained for a point and a planar source was carried out. In order to contribute to defects characterization studies, the influence of the crack's characteristics such as its size, shape and placement (depth and position) was analyzed using a phase contrast approach. Other features that may be relevant in IRT experiments, such as the nature of the stimulus provided and its distance from the surface were also studied. Analysing thermal pattern images obtained using infrared thermography (IRT) has shown to be an effective non-destructive testing (NDT) technique which is used in many sectors for many applications, including the detection of hidden defects. Defects appear as anomalies in the thermal patterns of thermographic images since their presence affects the heat and moisture diffusion phenomena. Passive IRT studies are performed with materials in their natural thermal state and are mostly done using a static approach. However, if a temperature gradient that allows the identification of anomalies in the thermal patterns is not naturally present, it may be necessary the use an additional heat source in order to produce it. This technique is known as active IRT. Additionally, if results are obtained in a transient regime, and the nature of the heat source generated in active IRT is well defined, a quantitative characterization of defects may be performed by solving heat transfer problems using thermographic data. For this reason, active IRT has been used in NDT in a great number of areas, including in civil engineering. In particular, the technique has been successfully used to test the integrity of composites and structures, having detected surface moisture and located defects in concrete composites up to a depth of about 10 cm, as reported by Wiggenhauser and Maierhofer (C. Serra, 2013).

Figure 1 is a general representation of the experimental apparatus for an active IRT test. A known thermal wave generated by a heat source (stimulus) is applied to a test specimen, leading to heat flow inside it. The reflected thermal wave is altered by defects inside the specimen, which produces disturbances in the temperature patterns on the surface. These are recorded by the IRT camera as a function of time. Data is stored in a computer and can then be subject to a range of processing techniques (data analysis).

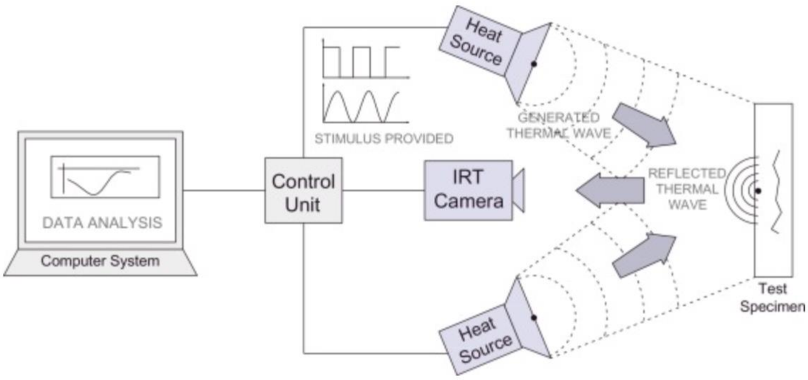


Figure 1 Schematic representation of an experimental setup for an active IRT

2.2. Agent-Based Modelling (ABM's)

It usually starts out with modeling properties and behavior of individual agents and only thereafter considers macro-level effects to emerge from the aggregation of agents' behavior. In ABM, the individual agent is the explicit subject to the modeling effort. With this, ABM offers an additional level of validation. Like EBM, it allows comparing model output with observed system behaviour. Additionally, however, it can be validated at the individual level by comparing the encoded behaviour of each agent with the actual behaviour of real agents. This, however, usually requires additional data, hence more efforts in empirical research (Barbati M, 2011).

Basically, ABM might seem intuitively more appropriate for modelling social systems since it allows and even necessitates considering individual decisions, dispositions, and inclinations. Its natural modularization follows boundaries among individuals, whereas in EBM, modularization often crosses these boundaries. What is more, ABM allows representing space, thereby offering possibilities to consider topological particularities of interaction and information transfer. In combination with graph theory and network analysis, it enables precise conceptualizations of differences in frequency, strength, existence, etc. of interactions between agents.

Agent-based modeling (ABMs) is a style of modelling in which we represent the interaction between individuals and with each other environment in a program. Agents can be, for example, people, animals, groups, or cells. They can model entities that do not have a physical basis but are entities that can perform some tasks such as gathering information or modeling the evolution (Asgari S, 2016).

It is a method of modeling complex systems by defining rules and behaviors for individual components (agents) as well as the environment they are present in. Further, we aggregate these rules to see the general behavior of the system. It helps in understanding how simple micro-rules of individual behavior emerge into macro-level behavior of a system. Being able to model these complex systems can lead to a better understanding of them, thereby being able to control the course of events, just by tweaking simple rules at the individual level (L, 2012).

Besides, reviews of ABMs in the context of ecology, environmental management, and land use include (Bousquet 2004; Matthews 2007; Grimm & Railsback 2005; Caplat 2008; DeAngelis & Diaz 2019). In some applications, interventions or treatments were addressed and therefore required the adaptation of agents to changing scenarios (Berry 2002).

ABMs have also been used to simulate epidemics with analyses examining the impact of implemented or potential intervention measures (e.g., quarantining/physical distancing, mask wearing, and vaccination) (Mniszewski 2013; Perez & Dragicevic 2009; Tracy 2018). Visual representations of epidemiological ABMs have even been used by news outlets during the COVID-19 pandemic to help explain to the public how various intervention methods change the shape of an epidemic (*i.e.*, "flatten thecurve) or the basic reproduction number (R_0) of an epidemic; see, for example, Fox (2020) and Stevens (2020).

3. Methodology

3.1. Research Data

This chapter discussed the research process, and the using of ABMs in life science courses and also in mathematics modelling courses. The aims of this chapter are to brief the methods used to carry out this study, how the study was designed, how it can be solved by using the relevant software.

3.2. Derivation of Heat Diffusion Equation

Equation below is the criteria that have on this simulation which is governing equation

$$\rho . \mathbf{c_p} \frac{dT}{dt} = k\left(\frac{d^2T}{dx^2} + \frac{d^2T}{dy^2} + \frac{d^2T}{dz^2}\right)$$

where, k is the material conductivity while ρ is density and $\mathbf{c_p}$ is the specific of heat capacity. In this section, we will see the formulation of the flow of heat diffusion through the model of rectangular shape. First, the heat equation will be derived in three dimensional. The heat equation is derived by implementing the physical principle of conservation of energy which state that

Rate of change of energy inside element	=	Net flux of heat into element	+	Rate of work done on element due to body and

or equivalently, let

A = B + C (1)

where A, B, and C are the respective terms. The C term is equal to zero by differences in temperature and hence there is no work done due to body forces and surface forces.

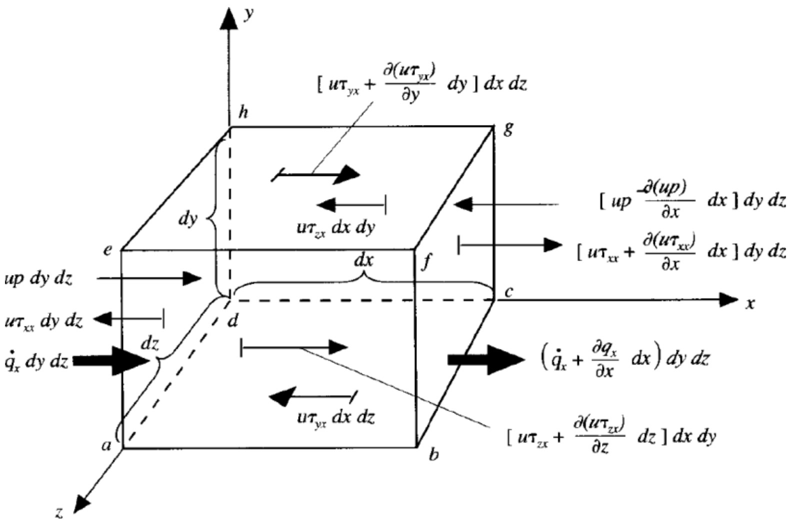


Figure 2 The energy fluxes in x-direction of the infinitesimal small, moving through model

Let's look at the B term which is the net flux of heat into the fluid element. Inthis case, the heat flux is due to the heat transfer by the temperature gradient across thesurface of fluid element. Let q_x denote the heat transferred in the x direction per unit time per unit area by thermal conduction. From Figure 2, the net heat transfer in the x direction into the fluid element by thermal conduction is

$$ux - \left(qx + \frac{\partial qx}{dx} dxL \right) dydz = \frac{\delta qx}{\delta x} dxdydz \qquad (2)$$

By considering also the heat transfer in the y and z directions through other faces, the B term is

$$B = -O \frac{\delta qx}{\delta x} + \frac{\delta qy}{\delta y} + \frac{\delta qz}{\delta z} P \; dxdydz \qquad (3)$$

According to Fourier's law of heat conduction proportional to the localtemperature gradient, the heat flux is

$$qx = -k \frac{\delta T}{\delta x} \qquad qy = -k \frac{\delta T}{\delta y} \qquad qz = -k \frac{\delta T}{\delta z}$$

where k is the thermal conductivity. Hence, Equation can be written as

$$B = pq \; \frac{\delta}{\delta x}\left(\frac{k\delta T}{\delta x}\right) + \frac{\delta}{\delta y}\left(\frac{k\delta T}{\delta y}\right) + \frac{\delta}{\delta z}\left(\frac{k\delta T}{\delta z}\right) dxdydz \qquad (4)$$

$$= k\frac{\delta T}{\delta x} + k\frac{\delta T}{\delta y} + k\frac{\delta T}{\delta z} \; Pdxdydz \; .$$

Now examine the A term which is the rate of change of energy inside fluid element. The energy in the fluid element includes internal energy and kinetic energy. However, in the case of heat transfer, the kinetic energy could often be neglected. Let denote E, the internal energy

$$E = \rho. dxdydz \,. cp \,. T \qquad (5)$$

where c_p is specific heat. Hence, the time rate of change of energy of amoving fluid element is given by the substantial derivatives.

$$A = \rho cp \frac{DT}{Dt} dxdydz \qquad (6)$$

This is also equal to

$$A = \rho cp\ K\frac{\delta T}{\delta t} + V.\nabla TL\ dxdydz$$

$$= \rho cpSV.\nabla Ttdxdydz$$

$$= \rho cp.K.u\frac{\delta T}{\delta x} + v\frac{\delta T}{\delta y} + w\frac{\delta T}{\delta z}\ dxdydz \qquad (7)$$

By substituting Equations (4) and (7) into Equation (1), the final form of heat energy equation is

$$\rho cpKu\frac{\delta T}{\delta x} + v\frac{\delta T}{\delta y} + w\frac{\delta T}{\delta z}L\ dxdydz = kO\frac{\delta T}{\delta x} + k\frac{\delta T}{\delta y} + k\frac{\delta T}{\delta z}Pdxdydz \qquad (8)$$

$$Ku\frac{\delta T}{\delta x} + v\frac{\delta T}{\delta y} + w\frac{\delta T}{\delta z}L = \frac{k}{\rho cp}.O.\frac{\delta T}{\delta x} + \frac{\delta T}{\delta y} + P\frac{\delta T}{\delta z} \qquad (9)$$

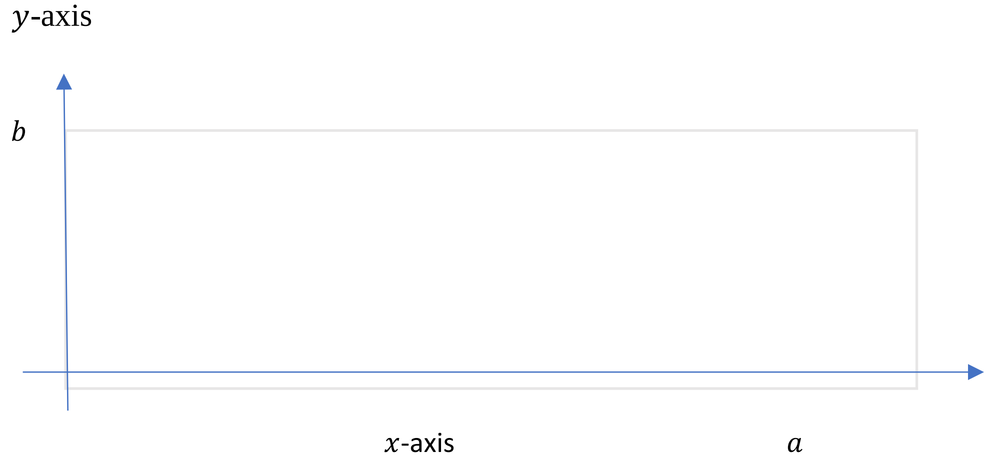
After rearrange, the heat energy equation to governing equation of the model flow driven by temperature differences is

$$\frac{k}{\rho cp}.O.\frac{\delta T}{\delta x} + \frac{\delta T}{\delta y} + \frac{\delta T}{\delta z}P - Ku\ \frac{\delta T}{\delta x} + v\ \frac{\delta T}{\delta y} + w\ \frac{\delta T}{\delta z}L \qquad (10)$$

So, we get the heat equation in form of three-dimensional. Now, we need to reduce on two-dimensional form since in this research was go through to the rectangular shape for model structure.

3.3. Mathematical of heat diffusion phenomenon

We assume the plate of rectangular shape, represented as $R = [0, a]x[0, b]$



$$\rho.\mathbf{c_p}\frac{dT}{dt} = k\left(\frac{d^2T}{dx^2} + \frac{d^2T}{dy^2}\right)$$

with the initial condition

$$u(x, y, t) = 0 \quad , \quad T = 0$$

and the boundary condition

$$u(x, y, t) = 20 \quad , \quad T = 100$$

3.4 Modelling Heat Diffusion phenomenon by ABM

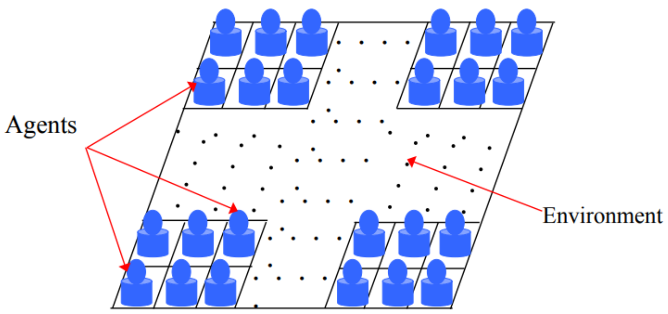


Figure 3 Conceptual model of heat diffusion phenomenon by ABM

From the Figure 3, there are some criteria that must have in agent-based modelling situation. First is environment, which is in two-dimensional space and divided into cells. Then, each of the cells is a fix agent model.

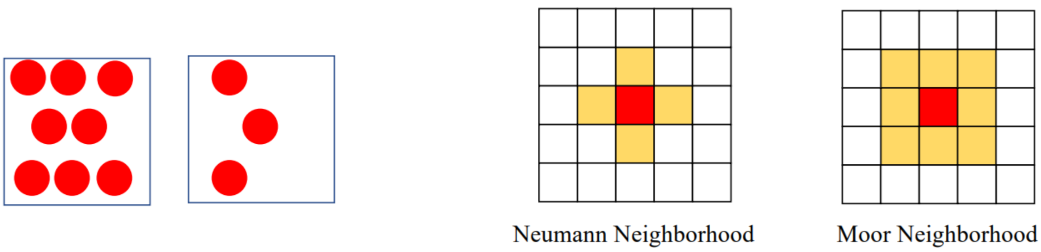


Figure 4 Agents and environment

A neighborhood is an area where people live and interact with one another. Neighborhoods tend to have their own identity, or "feel" based on the people who live there and the places nearby. Residents may have similar types of families, incomes, and education level. Neighborhoods can include restaurants, bookstores, and parks.

Neighborhoods often have fuzzy geographical boundaries, so sometimes it's difficult to tell where one starts and another ends. So, this term was applied in agent-based modelling which affects the temperature of specific cell or agent. On Figure 4, neighborhood have two types which is Neumann and Moor Neighborhood.

4. Results and discussion

4.1. Result in Netlogo

Figure below show the result of two-dimensional plate of rectangular shape (using wood as material type) in Netlogo software. As we can see, it has different part of temperature. Besides, we also can see that the movement of heat from cold end and hot end.

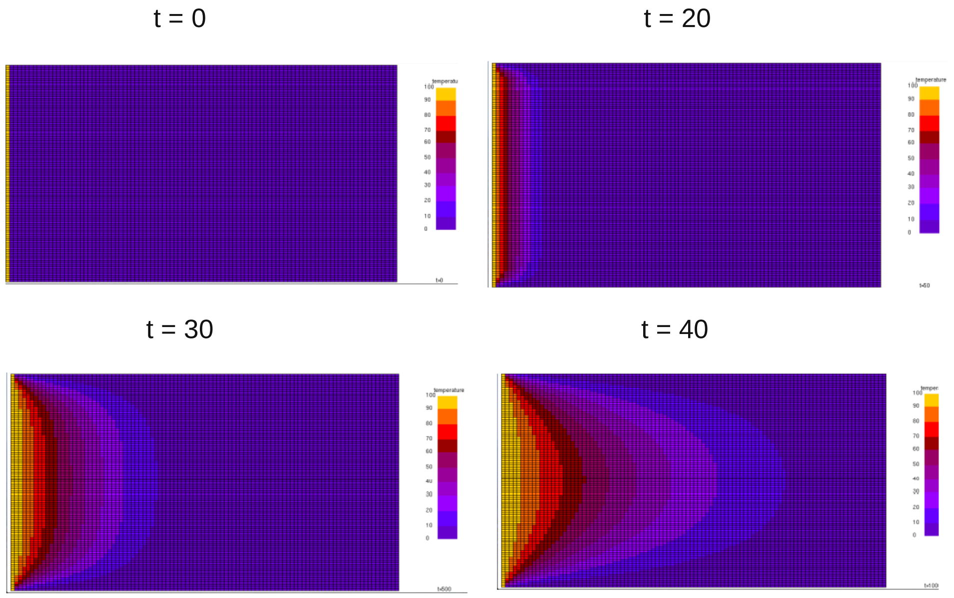


Figure 5 The flow of heat diffusion in different time

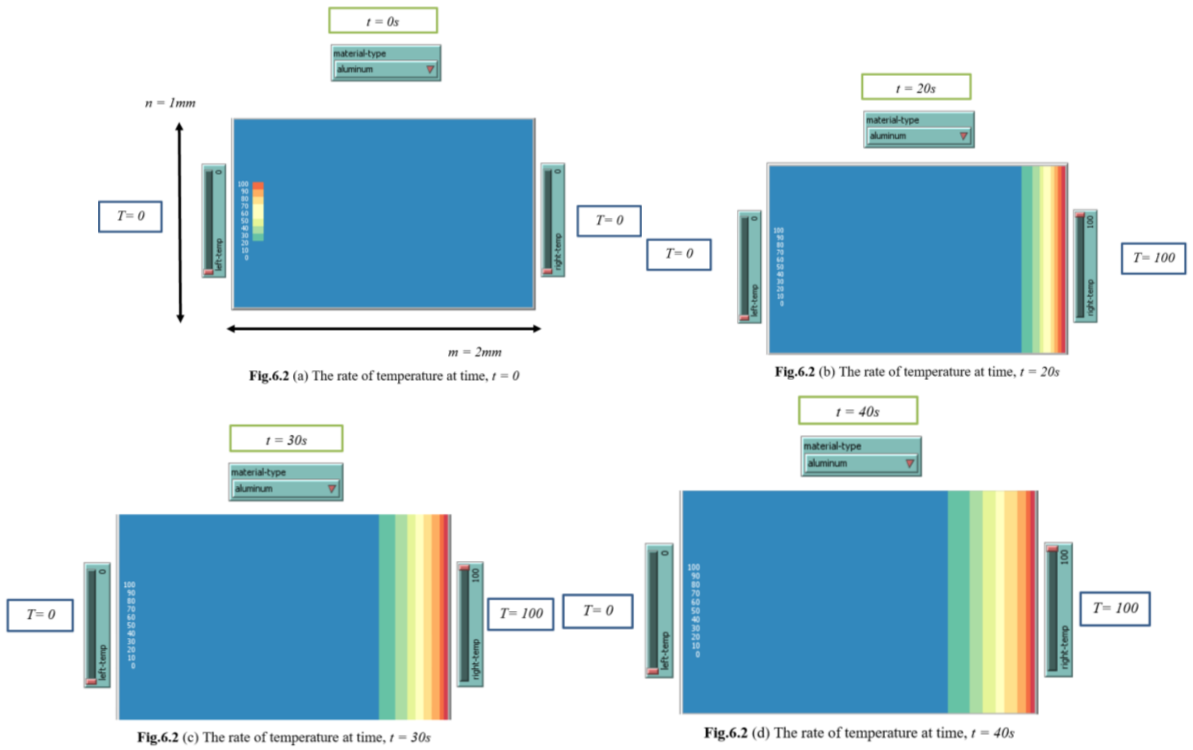


Fig.6.2 (a) The rate of temperature at time, *t = 0*

Fig.6.2 (b) The rate of temperature at time, *t = 20s*

Fig.6.2 (c) The rate of temperature at time, *t = 30s*

Fig.6.2 (d) The rate of temperature at time, *t = 40s*

Fig 6.2(a), 6.2(b), 6.2(c) and 6.2(d) above showing the rate flow of heat in different boundary of time and temperature.

4.2. Result in COMSOL Multiphysics

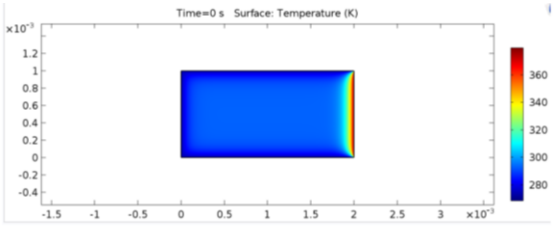


Fig.6.3 (a)

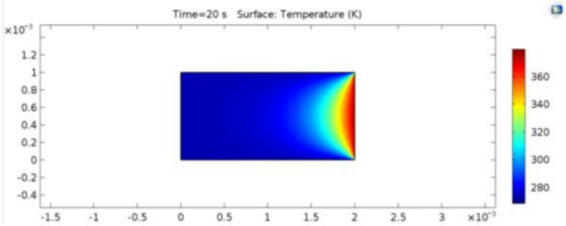


Fig.6.3 (b)

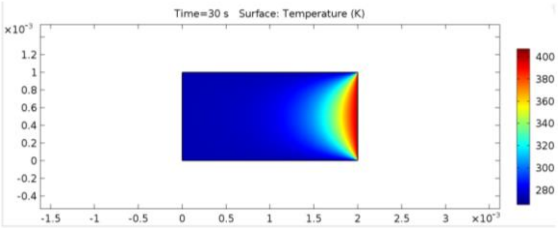


Fig.6.3 (c)

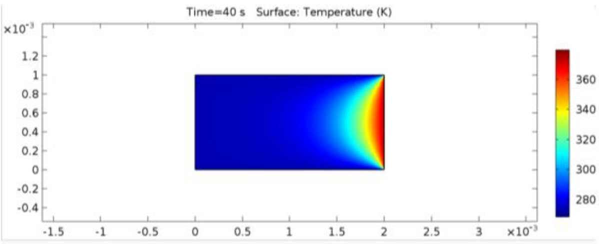


Fig.6.3 (d)

Fig 6.3 (a), Fig 6.3 (b), Fig 6.3 (c), and Fig 6.3 (d) show model of rate flow of simulation heat diffusion phenomenon in rectangular shape for the time at *t = 0s, t = 20s, t = 30s, and t = 40s* respectively.

For this part, the structure of the model in this software was done to investigate the flow of heat from hot end to cold end with a boundary condition (time and temperature).

4.3. Comparison of numerical method between Netlogo and COMSOL Multiphysics software

The comparison that can see through both software is Netlogo can produce a movement of particle with a specific when COMSOL Multiphysics. Even though COMSOL Multiphysics cannot produce it, but that software can measure variety of any criteria such as temperature, time, boundary condition, and another mathematic measurement. Next, for measuring a material, from my research are easier to use COMSOL Multiphysics to measure the material. In addition, in COMSOL Multiphysics are already given any material that we want to put like copper, aluminium, rod and another.

Besides, in Netlogo have no limit time to measure the movement the particle. It means that, in that software was suitable to measure from begin until the end of the movement of particle.

Conclusion

The study's goal was met throughout the process, and an appropriate model of heat diffusion that was created. A heat diffusion model has been structured to investigate the flow of heat through the a two-dimensional of rectangular shape. With addition, the rectangular model was used in a software to develop a heat flow with a condition on it. As a result, it concludes all chapters in this chapter with some limitations from this study and some recommendations for future research.

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