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Modelling for Extraction of Major Phytochemical Components from *Eurycoma longifolia*

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Abstract: A mass transfer model of major phytochemical components from *Eurycoma longifolia* was developed in order to describe the solid-liquid extraction process. The yield of the extraction normally depends on the operating parameters such as solvent to raw material ratio, extraction time, temperature and agitation speed. In this study, the model was developed taking into account the two-way mass transfer of solute into liquid phase and the solvent into solid system. The influence of processing variables such as extraction temperature, solvent to raw material ratio and agitation speed was simulated by the model. Several assumptions were made in the theoretical approach to solve the simulation algorithm in order to predict the performance of the solid-liquid extraction system. From the study, it can be concluded that when the extraction temperature was increased, the yield of extraction also increased and this has reduced the extraction time. The best agitation speed was found to be at 400 rpm.

Key words: *Eurycoma longifolia*, phytochemical, mathematical model, mass transfer, solid-liquid extraction

INTRODUCTION

The herbal industry in Malaysia was reported to have achieved an annual sale of more than RM4.5 billion and the figure is expected to double by 2010. This represents a vast opportunity for industries within Malaysia especially in view of the fact that Malaysia has the 12th largest biodiversity in the world, with 1200 plants species recorded as having medicinal value (Aziz, 2003). Malaysia is endowed with rich rain forests which comprise thousands of plants with potential medicinal values. One such plant is the tall shrub tree from the Simaroubaceace family, *Eurycoma longifolia* known locally as Tongkat Ali which is commonly found along the hilly jungle slopes of Malaysia. This plant is well-known in several regions of South East Asia for its high medicinal values. It has been promoted as the Malaysian ginseng due to its aphrodisiac effects (Shafiqul *et al*., 2006).

Traditionally, Tongkat Ali is valued for its aphrodisiac properties and treatment of diverse ailments ranging from cuts and wounds, skin infection, fever, malaria, high-blood pressure, diabetes to increased energy and stamina. In Malaysia, research has confirmed that isolated constituents as well as whole plant extract show aphrodisiac, anti-malarial, anti-tumor or cytotoxic properties, anti-ulcer and antiviral activity.

Research conducted at Universiti Sains Malaysia has shown that Tongkat Ali has anti-malarial property that is stronger than chloroquinine (Ang *et al*., 2002).

There are two specific challenges in herbal and phytochemical processing. The first challenge is to increase product yield while maintaining overall process reasonable economics and secondly is to produce or achieve a standardized extract with the active ingredients available in the desired concentration and profile. Tongkat Ali requires a longer time to produce the secondary bioactive metabolites and their biological activities may be derived from more than one of the constituents. The phytochemical content in herbs is extremely low and losing a small fraction of the desired extract is significant in terms of extraction yield. If yield can be increased, it would increase profitability.

Current yield of Tongkat Ali achieved was in between 3 to 4%. However, an increase of production of even 0.5% in weight could increase profits by up to 20%. The current selling price of Tongkat Ali water extract spray dried powder is at RM 2000 to RM 3000 per kg which converts to approximately RM 20,000 per kg in capsule form. Therefore, there is a strong incentive to optimize production yield (Kaur, 2003).

Tongkat Ali holds a vast potential and value for commercial production in health and wellness industry

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based on these traditionally benefits and scientifically proven properties. Therefore, it is necessary to study in depth the effects of the processing parameter such as extraction temperature, solvent to raw material ratio and agitation speed to the yield of production. In *Eurycoma longifolia* production, the yield of bioactive constituents is extremely low. In this study, a mathematical model of *Eurycoma longifolia* extraction was presented that predicts the extraction of major phytochemical components. The model was developed to improve the extraction process in order to increase the yield of major phytochemical components. The parameters in the model were estimated using previous experimental data. The effects of operating conditions such as temperature, solvent to raw material ratio and agitation speed on the yield of effective compounds were investigated through the model simulation.

MATERIALS AND METHODS

- The work was divided into two main phases
- Development of mathematical model
- Simulation and validation of the model

Development of mathematical model: A mathematical model was developed for extraction of major phytochemical components from *Eurycoma longifolia*. Three major compounds from *Eurycoma longifolia* were considered in this work which were eurycomanone, eurycomalactone and 14,15-β hydroklaineanone.

Tongkat Ali root chips were boiled in water in a pressurized vessel between 100 to 120°C for approximately 2 h during the extraction process. This boiling operation was maintained for 2 h to provide sufficient time for the phytochemical components in the root chips to be leached into the extraction solvent (water). Then, the boiled extract was run through a filter system where the water extract was separated from the solid particles. Approximately 35% of the solvent (water) was absorbed in the discharged chips and this was taken as process losses.

Mass and energy balance were performed. The degree of freedom must be zero in order to solve the system. The extraction consists of two major unit operations which are extractor and filter system. Overall mass balance for the system can be expressed as:

$$\frac{d(\rho V)}{dt} = \rho_1 F_1 + \rho_2 F_2 - \rho_4 F_4 - \rho_5 F_5 \qquad (1)$$

where, F_1 is the inlet flow rate to the extractor; F_2 is the inlet flow rate for solvent; F_4 is the outlet flow rate of liquid extract from filter and F_5 is the outlet flow rate of solid waste from filter.

For the energy balance, the equation is:

$$Q_{acc} = Q_{ag} - Q_{sen} \qquad (2)$$

where, Q_{acc} is the heat accumulation rate by the system, Q_{ag} is the heat generation due to mechanical agitation and Q_{sen} is the rate of sensible enthalpy gain by the flow system streams (exit-inlet).

$$Q_{acc} = \frac{dE}{dt} = \frac{d}{dt}[\rho V c_p (\Delta T)] \qquad (3)$$

where, E represents the energy accumulated in the system. ρ is the density of solution, V is the solution volume, c_p is the heat capacity and ΔT is the temperature difference between the temperature in the system and the reference temperature.

Assuming that ρ, c_p and T_{ref} are constant with respect to time:

$$Q_{acc} = \frac{dE}{dt} = \rho V c_p \left[V \frac{dT}{dt} + (T - T_{ref}) \frac{dV}{dt} \right] \qquad (4)$$

The extraction process from herb can be described in the following stages:

- The solvent must be transferred from the bulk solvent solution to the surface of the solid
- The solvent must penetrate or diffuse into the solid
- The solute dissolves into the solvent
- The solutes then diffuse through the solid solvent mixture to the surface of the particle
- The solute is transferred to the bulk solution

The extraction of phytochemical compounds from the herb is in nature, a mass transfer process of solute from the herb body to the solvent. Phytochemical compounds exist in the cells of the herb which makes the herb leaching process difficult and complex. The leaching rates of phytochemical compounds are dominated by the diffusion rates. Therefore, the mathematical model for the solid-liquid extraction process focuses on the diffusion process of the phytochemical compounds, which consists of diffusion to the surface of the herb from the inside particle and then move to the bulk solution.

There are two fundamental concepts that define *Eurycoma longifolia* extraction process which are the equilibrium and mass transfer rate (Cacace and Mazza, 2003). The diffusion model inside herb for eurycomanone can be expressed as follows:

$$\frac{dM_{A1}}{dt} = k_1A_1[C_{A0} - C_{A1}] \tag{5}$$

where, M_{A1} is the concentration of eurycomanone transferred across the cell membrane; k_1 is the overall mass transfer coefficient; C_{A0} and C_{A1} is the concentration of eurycomanone inside and outside the cell and A_1 is the area across which diffusion occurs. Equation 5 is also used for compound B for eurycomalactone and compound C for 14,15-β hydroklaineanone.

The overall mass transfer coefficient, k_1 can be written as follows:

$$k_1 = \frac{1}{\frac{1}{\alpha_1} + \frac{1}{\alpha_2}} \tag{6}$$

where, α_1 is the mass transfer coefficient of phytochemical compounds across the liquid near the cell membrane and α_2 is the mass transfer coefficient across the cell membrane.

For the diffusion model from the surface of the herb to the bulk solution as the following:

$$\frac{dM_{A2}}{dt} = k_2A_2[C_{A1} - C_{A2}] \tag{7}$$

where, M_{A2} is the concentration of eurycomanone transferred from the surface of the herb to the bulk of the solution; k_2 is the overall mass transfer coefficient; C_{A2} is the concentration of eurycomanone in the bulk solution and A_2 is the interfacial area between the particle and the liquid which can be approximated by the area of the herb particle absorbing the solvent. Equation 7 was used for compound B and C by substituting compound A with compound B and C.

In contrast, when the solution was agitated, the mass transfer coefficient is related to the Reynolds number and the Schmidt number by the following Eq. 8:

$$Sh = 0.33(Re)^{\frac{1}{2}}(Sc)^{\frac{1}{3}} \tag{8}$$

where, Sh is the Sherwood number represented by $Sh = k_2\delta/D$; Re and Sc are Reynolds number and Schmidt number and δ is the characteristic length.

The following general assumptions were made when developing the mathematical model:

- Solid particles were considered as spheres with a radius R and the effective constituents are initially uniformly distributed in the spheres
- The solvent was perfectly mixed. So the transfer resistance in the liquid phase was negligible and the concentration of the effective constituents in the solvent only depends on time
- The transport of the effective constituents in the particles was a diffusion phenomena and can be described by a diffusion coefficient (D) independent of time
- The diffusion of the effective constituents was carried out parallel and there was no interaction between them
- There was no adsorption of solute by the solid in the leaching process

It was found that the rate of extraction increases with extraction temperature until a certain temperature where increment in yield of extraction diminished. Extraction yields declined due to the degradation of temperature sensitive compounds. By increasing extraction temperature, the higher solubility of solute resulted in the increase of diffusion rate and thus increases the diffusion coefficient. This has reduced the extraction time. The effect of temperature was modeled using the Arrhenius type of relationship as shown in Eq. 9:

$$D = Ae^{Ea/RT} \tag{9}$$

where, D is the diffusivity of solute in the solid; E_a is the activation energy for diffusion; R is the Universal Gas Constant and T is the absolute temperature.

For the diffusion coefficient of solute in the liquid solvent, the effect of temperature used was the equation introduced by Wilke-Chang as shown in Eq. 10. Similarly, high temperature decreased the solvent viscosity and increased the diffusion coefficient.

$$D = 1.173x10^{-16}(\Phi M_E)^{\frac{1}{2}} \frac{T}{\mu_E {V_A}^{0.6}} \tag{10}$$

where, M_B is the molecular weight of solvent; T is the absolute temperature; μ_B is the viscosity of solvent; V_A is the molar volume of solute at the normal boiling point ($cm^3\ mol^{-1}$) and Φ is the association factor of solvent.

Simulation and validation of the model: Equation 5 and 7 which represented the mass transfer model for *Eurycoma longifolia* extraction process involves some differential equations. The model was simulated using Matlab programming environment. The differential equations were solved using Fourth-Order Runge-Kutta algorithm. The work by Athimulam *et al.* (2006) was used as the benchmark for the simulation study and the kinetic parameters were based on their work. The effect of extraction temperature on the yields of phytochemical compounds was investigated by varying the operating conditions individually. The effect of extraction ratio and agitation speed was also investigated.

RESULTS AND DISCUSSION

Effect of temperature on the yield of extraction of *Eurycoma longifolia*: The results shown in Fig. 1 are the comparison between simulation and experimental data. The extraction temperature studied was in the range of 60 to 110°C. It can be seen from Fig. 1 that the yield of extraction increased by increasing the extraction temperature but the yield decreased when the extraction temperature reached 100°C which is the boiling point for water as the solvent for the extraction process.

Heat treatment was performed to accelerate the mechanism of the diffusional process when extracting from plants. The surface tension and viscosity of the solvent reduced and the solvent reached the active sites inside the matrix more easily at higher temperature. In addition, high temperature can decrease the cell barrier by weakening integrity of the cell wall and membrane. As a result, the solvent can easily get in contact with phytochemical compounds. The temperature effect on the extraction yield came from its influence on diffusion phenomena.

An increase in temperature from 60 to 110°C increased the yield of extraction and reduced the extraction time. However, further increased of temperature from 100 to 110°C resulted in lower extraction yield. This was due to degradation of phytochemical compounds. Increasing temperature favored extraction by increasing the diffusion coefficient which increased the extraction rate.

Effect of solvent to raw material ratio on the yield of extraction of *Eurycoma longifolia*: The final yield was plotted as the function of water to Tongkat Ali ratio as shown in Fig. 2. From Fig. 2, the increment of extraction yield becomes insignificant when ratio was increased beyond 5:1. When the ratio increases, extraction yield increases until it reaches ratio 5:1. The higher the ratio of water to Tongkat Ali, the higher the difference of concentration between the bulk solution and the solutes. Therefore, more phytochemical can diffuse out if a higher volume of water is used. The synergetic effect of the phytochemical components that comes out of the sample has longer contact time with water may cause the decrease of extraction yield for ratio 7:1.

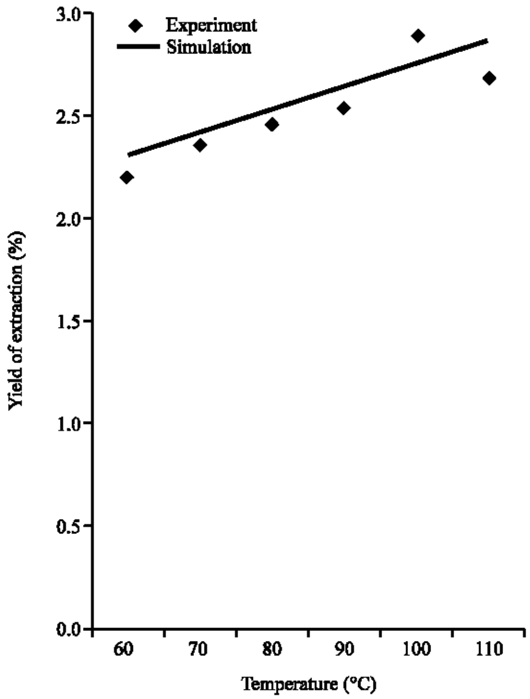

Fig. 1: Effect of temperature on the yield of extraction of *Eurycoma longifolia*

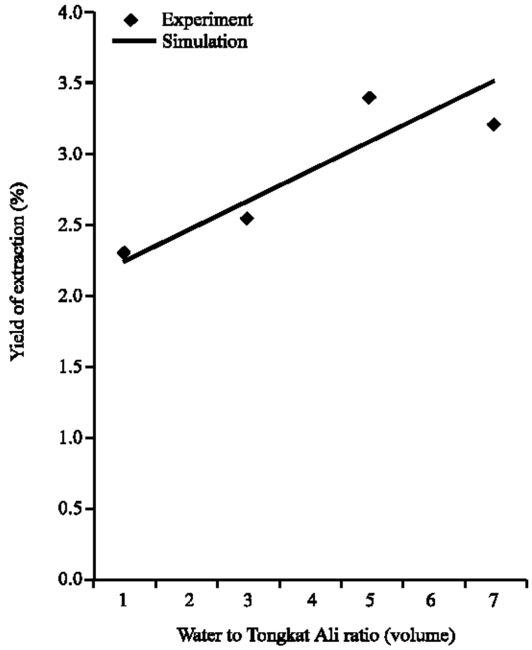

Fig. 2: Effect of water to Tongkat Ali ratio on the yield of extraction of *Eurycoma longifolia*

Effect of agitation speed on the yield of extraction of *Eurycoma longifolia*: From Fig. 3-5, the effect of agitation speed was studied at 100, 200 and 400 rpm. The

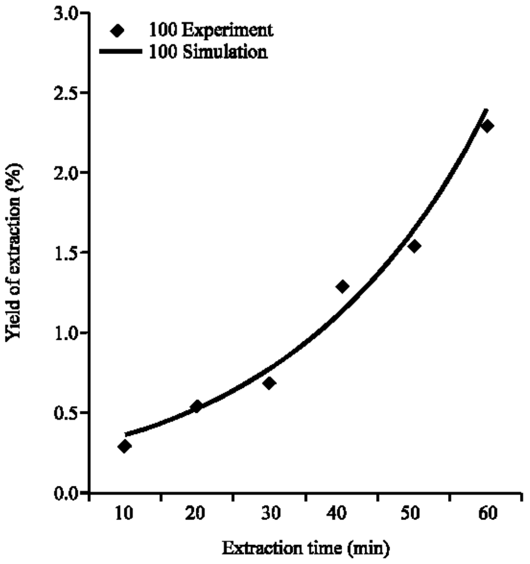

Fig. 3: Effect of agitation speed at 100 rpm on the yield of extraction of *Eurycoma longifolia*

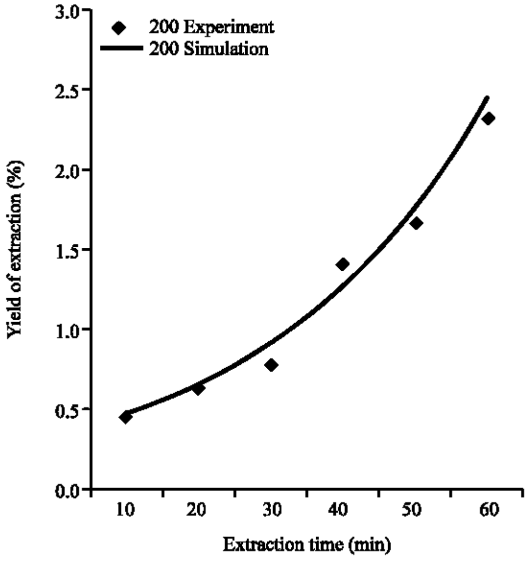

Fig. 4: Effect of agitation speed at 200 rpm on the yield of extraction of *Eurycoma longifolia*

best agitation rate was found to be at 400 rpm. When the solution is agitated, mass is transported by the bulk motion of the fluid which known as convective mass transfer. Convective mass transfer occurred at the surface when a fluid is outside the solid. Therefore, when the agitation speed increases, the Reynolds number is also increased. The Reynolds number is related to the mass transfer coefficient. So, the higher the Reynolds number, the higher the mass transfer coefficient.

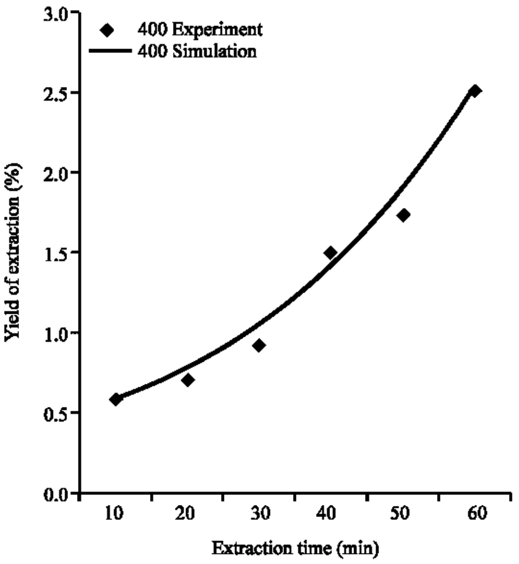

Fig. 5: Effect of agitation speed at 400 rpm on the yield of extraction of *Eurycoma longifolia*

CONCLUSION

A good fitting between experimental data and the model was obtained. The work concluded that when extraction temperature was increased, the yield of extraction also increased and this has reduced the extraction time. The best agitation speed was found at 400 rpm. The yield of extraction will increase when the ratio of water to Tongkat Ali increases until 5:1 ratio. Further work will be carried out to determine the optimum operating conditions such as extraction time.

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