*Mj. Int. J. Sci. Tech.* **2009**, *1*(Special Issue), 85-94

Maejo International
Journal of Science and Technology
**ISSN 1905-7873**
Available online at www.mijst.mju.ac.th

*Full Paper*

# Sensitivity of produce respiration models used in the MAP-DESIGN software on the shelf life simulation of broccoli in the modified atmosphere package

**Weerasak Lertsiriyothin**

School of Agricultural Engineering, Institute of Engineering, Suranaree University of Technology,
Nakhon-Ratchasima 30000, Thailand

E-mail: LSRYTW@sut.ac.th

*Received: 17 July 2008 / Accepted: 13 January 2009 / Published: 22 January 2009*

---

**Abstract:** Optimization for the designing of modified atmosphere packaging (MAP) for broccoli was made by the MAP-DESIGN software (author's own code). The software is capable of dealing with all parameters required for the designing of MAP for fresh produce, namely packaging materials, package dimensions, storage conditions, and plant respiratory models. Computational algorithms were carefully designed based upon widely-used theories of living plant respiration, gas permeability through packaging film, and heat transfer. Here, the effect of respiration models on the variation of shelf life estimation was evaluated by using broccoli in the MAP as the product sample. The computational results of product shelf life showed that the choice of respiration models, including a transition state model and an enzyme kinetic model, had a strong impact on the accuracy of shelf life estimation. A shelf life prediction of broccoli in MAP also revealed that the package dimension had little effect on time to reach steady-state condition, but had a significant effect on the level of $O_2$ remaining inside the package at equilibrium. A validity of shelf life prediction was tested against the previous experimental data of broccoli shelf life in a selected MAP.

**Keywords**: MAP-DESIGN software, modified atmosphere packaging, shelf life

---

## Introduction

A short shelf life for the products of fresh vegetables and fruits is notorious among fresh produce producers. Therefore, all producers have been competing to find a way of extending the shelf life in the hope of cutting the production cost. One of the widely applied techniques is by using modified atmosphere packaging (MAP) together with a cold storage condition. Even though the MAP method has been known for a long time, the technique has a limited use in certain groups of vegetables or fruits due to a lack of all-purpose packaging film and also of accuracy of plant respiration and transpiration predictive models. The latter issue is considered as a big hurdle since the models need to incorporate a function of storage variables, e.g. humidity, temperature and air composition. Currently, there are only three respiration models used for the MAP DESIGN, namely constant rate respiration model, enzyme kinetic model [1-2], and transition state model [3]. The only model that is a true function of temperature was the transition state model whereas the first two models must rely on Arrhenius function to predict the effect of temperature on the respiration rate. Nevertheless, all the three models require a specific group of parameters based on an actual measurement of plant respiration.

The other hurdle is related to the designing of MAP for the products for which the process involves a lot of computation. The computation must simultaneously consider all factors, i.e. plant respiration, packaging constraints and storage conditions. Since each of the factors contains tremendous data and variables, the computational protocol to predict the shelf life frequently becomes a cumbersome process. Perhaps this may be the main reason for a slow improvement on the MAP technology.

In order to accelerate the design process, the "MAP DESIGN" software for fresh vegetables or fruits has been created [4]. The "MAP DESIGN" is capable of handling all design factors needed by the packaging engineer. The objective of this paper is to demonstrate the effect of plant respiration model on the rate of change of the gas composition ($O_2$, $CO_2$) inside the modified atmosphere package as predicted by the MAP DESIGN software.

### *Design Concept*

The MAP DESIGN software has been developed for the packaging engineer to use as a tool in the designing of modified atmosphere packaging for fresh vegetables or fruits. Designing means that the software must be capable of predicting the shelf life of packed fresh produce as a function of all major constraint conditions given by the designer. These constraint conditions include packaging material specification, specifically packaging size or dimension, and an exposed environment. Thus, this concept is accomplished by structuring the program to cope with designer questions which are divided into three main categories, namely a choice of plant respiration models, environmental conditions (storage and handling scenario), and packaging parameters. To make the MAP DESIGN software becomes the true high-end software; the MAP software is created to have a mode of user-defined function values for all mentioned constraint conditions. The benefit of this mode increases the feasibility of the MAP DESIGN software to be used in the designing work.

*Plant Respiration Models*

-*Constant rate model*: The respiration rate is treated as a function independent of $CO_2$ or $O_2$ level. The rate value at a given temperature is extracted from the database of respiration rates which are recorded at various temperature values by using a non-linear interpolation method. In the MAP software, the respiration rate is automatically provided when the type of plant and storage temperature are assigned.

-*Enzyme-kinetic model*: The respiration rate model is described by Michaelis-Menten equation. The $O_2$ consumption rate and $CO_2$ evolution rate are separately modeled as a function of changing concentrations of $CO_2$ and $O_2$, as shown in the following equations [2]:

$$R_{O_2} = \frac{V_{m1}[O_2]_i}{K_{m1} + [O_2]_i + \{[O_2]_i[CO_2]_i\}/K_{i1}} \qquad (1)$$

$$R_{CO_2} = \frac{V_{m2}[O_2]_i}{K_{m2} + [O_2]_i + \{[O_2]_i[CO_2]_i\}/K_{i2}} \qquad (2)$$

Where: $V_{m1}$ = $O_2$ coefficient for $O_2$ consumption rate, $K_{m1}$ = %$O_2$ for $O_2$ consumption rate, $K_{i1}$=%$CO_2$ for $O_2$ consumption rate, $V_{m2}$= $CO_2$ coefficient for $CO_2$ evolution rate, $K_{m2}$= %$O_2$ for $CO_2$ evolution rate, and $K_{i1}$ =%$CO_2$ for $CO_2$ evolution rate. All variables appearing in the equations 1 and 2 have to be obtained by actual measurement of respiration rate at any given constant temperature.

-*Transition state model*: Makino et al. [3] developed a temperature-dependent respiration rate model for fresh produce by using a transition state theory. The group proposed an $O_2$ consumption rate model which was proved satisfactory for various fresh produce [3, 5-6], as demonstrated below:

$$R_{O_2} = \frac{abp_{O_2}}{1 + ap_{O_2} + aip_{O_2}p_{CO_2}} \qquad (3)$$

Where: $a$ , $i$ = rate parameters [$kPa^{-1}$], $b$ =maximum $O_2$ consumption [$mol.kg^{-1}.s^{-1}$], $p_{O_2}$ , $p_{CO_2}$ = partial pressure of $O_2$ and $CO_2$ surrounding the fresh produce [kPa]. The parameters *a, b* and *i* are specific for a type of produce and are evaluated from the data of actual respiration measurement. Methodology details were clearly provided in the above cited articles.

The $CO_2$ evolution rate was obtained by a respiration quotient:

$$R_{CO_2} = RQ \times R_{O_2} \qquad (4)$$

Where: $RQ$ = respiratory quotient.

### *Packaging Design Models*

*-Gas transfer model:* Modified atmosphere packaging for fresh produce means an optimum condition of gas composition and energy level for extending the product shelf life. A prolonged shelf life happens because the rate of deterioration can be slowed down as a result of respiration control [7]. Normally, the optimum conditions are used to decrease the rate of respiration in order to minimize the biological activity. To control the gas combination, the gas transfer mechanism must rely on the permeability property of packaging material and surrounding conditions. Differential equations of the gas transfer models used for computation of the gas level are presented below:

$$\frac{dn_{O_2}}{dt} = \frac{P_{O_2} A\left(p_{O_2,out} - p_{O_2,in}\right)}{L} - R_{O_2} M \qquad (5)$$

$$\frac{dn_{CO_2}}{dt} = R_{CO_2} M - \frac{P_{CO_2} A\left(p_{CO_2,in} - p_{CO_2,out}\right)}{L} \qquad (6)$$

Where: $P_{O_{2,in}}, P_{CO_{2,in}}$ = partial pressure of $O_2$ and $CO_2$ inside the package [Pa], $P_{O_{2,out}}, P_{CO_{2,out}}$ = partial pressure of $O_2$ and $CO_2$ outside the package [Pa], $A$ = packaging surface area [$m^2$], $L$ = packaging film thickness [m], $M$ =produce mass [kg], $\frac{dn_{O_2}}{dt}$ = the derivative of $O_2$ amount with respect to time inside the package [mol/s], $\frac{dn_{CO_2}}{dt}$ = the derivative of $CO_2$ amount with respect to time inside the package [mol/s], $R_{O_2}$ = $O_2$ consumption rate [$mol.kg^{-1}.s^{-1}$], and $R_{CO_2}$ =$CO_2$ evolution rate [$mol.kg^{-1}.s^{-1}$].

*-Energy model:* Energy model is a vital expression because it has a tremendous impact on the accuracy of the simulation process. Any error occurring in the predictive temperature change of the product gets carried over to the computation of gas composition, specifically the moisture level inside the modified atmosphere package. The energy equation contained in the "MAP DESIGN" software is derived from the energy conversation law by taking account of all related energy forms, namely respiration heat and surrounding energy. Unfortunately, details of this part cannot be provided at this point of time due to protection of licensing rights.

## Materials and Methods

### *Sample and package*

*-Fresh produce:* Broccoli (unspecified variety) was selected as a testing produce based on the fact that its respiration models were reported by various research teams [5,8]. All of the respiration parameters for each model were assumed accurate and used for the simulation without any change. Therefore, the data of respiration models also served as an unprejudiced comparison. However, various cutting size of broccoli for the determination of respiration rate were found among the research teams and definitely had an influence on the accuracy of respiration rate prediction. Even so, there was no report of how severe that effect has on the predicted shelf life of fresh produce packed in the MAP.

Thus, the effect of product size is an objective of this work. Here, sample size used in the simulation was assumed in a form of small pieces, but not in a finely chopped form. A 0.5 kg of sample was filled in the package for every numerical simulation case. All constant parameters of the tested respiration models for broccoli were given as follows:

Enzyme kinetic model: $O_2$ consumption; $V_{m1}= 5.84\times10^{-5}$, $K_{m1}=0.6$, and $K_{i1}=2.3$,

$CO_2$ evolution; $V_{m2}= 6.53 \times 10^{-5}$, $K_{m2}=1.7$, and $K_{i2}=1.93$

Transition state model: $a=5.48\times10^{-4}$, $b=1.80\times10^{-6}$, $i=5.69 \times 10^{-5}$, and RQ=1

-*Package:* Flexible bags made of 45 micron Orega® film (low density polyethylene and 5% zeolite) were used as sample packages. The gas permeability coefficients of the film at 15 °C were $6.84\times10^{-16}$, $2.56\times10^{-15}$, and $1.23\times10^{-15}$ $mol.m^{-1}.s^{-1}.Pa^{-1}$ for $O_2$, $CO_2$ and $H_2O$ respectively. Bag volume and surface area were 0.0005 $m^3$ and 0.069 $m^2$ respectively. The void volume of the air inside the package was determined by subtracting the produce volume from the air-filled bag volume.

### *Simulation methods*

-*Simulation software:* The "MAP DESIGN" software (author's own code) [4], developed by using the Microsoft Visual C#.net language, was used in this work. By virtue of the Microsoft Visual language, all input parameters were created in the form of window base, and all database and computational results could be interfaced to the Microsoft Access. All computational procedures were carried out by using highly accurate numerical methods. A choice of user-defined error on the computational part was not provided since computational time was not a problem in the problem solving method. On the other hand, the computational program was set to handle the maximum possible numerical digits.

-*Simulation conditions:* The initial conditions for the simulation were set as follows: initial concentration of $O_2$ inside the bag= 20%, initial concentration of $CO_2$ inside the bag = 0.04 %, initial relative humidity of the inside and outside air = 10%, storage temperature= 15 °C, and heat transfer coefficient of the air inside and outside the bag = 1 W/m.K.

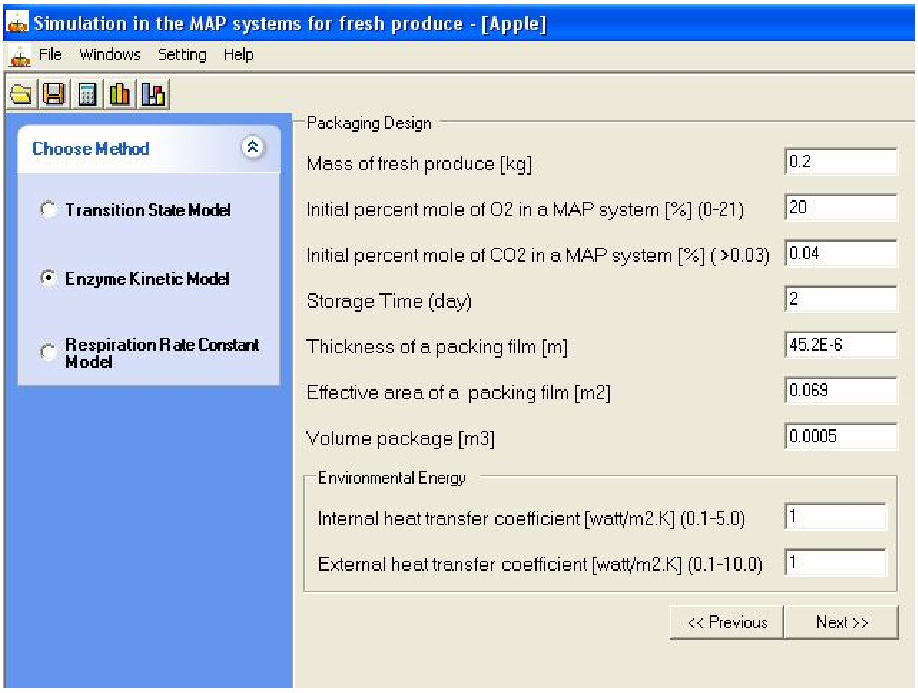
## Results and Discussion

### *Overview of the "MAP DESIGN" software*

All command functions appearing in the "MAP DESIGN" software were created in the form of window base, e.g. a packaging design window as shown in Figure 1, thus allowing the user to be guided through each step of commands as requested by the software without any difficulty. Besides, the "MAP DESIGN" was equipped with database of all design parameters ready for use if the designer preferred not to give the input himself. The validation details for the simulation codes used in "the MAP DESIGN" were given elsewhere [9].

*Effect of respiration model on the simulation of gas composition*

The effect of respiration model on the simulation of the rate of change of gas composition inside the package was tested by setting a constant set of all parameters, except for the choice of respiration consisting of environmental conditions (i.e. storage temperature, humidity, heat transfer coefficient), packaging parameters (i.e. type of flexible film, dimension), and mass of produce.



Choose Method

○ Transition State Model

● Enzyme Kinetic Model

○ Respiration Rate Constant Model

Packaging Design

Mass of fresh produce [kg]: 0.2

Initial percent mole of O2 in a MAP system [%] (0-21): 20

Initial percent mole of CO2 in a MAP system [%] ( >0.03): 0.04

Storage Time (day): 2

Thickness of a packing film [m]: 45.2E-6

Effective area of a packing film [m2]: 0.069

Volume package [m3]: 0.0005

Environmental Energy

Internal heat transfer coefficient [watt/m2.K] (0.1-5.0): 1

External heat transfer coefficient [watt/m2.K] (0.1-10.0): 1

**Figure 1.** A window of "Packaging Design Option" in the "MAP DESIGN" software

For this testing, a 0.5 kg of broccoli was packed in a 0.5 L of Orega® bag, which was then filled with ambient air and stored at a constant temperature of 15 °C and relative humidity of 10%. The rate of change of gas composition inside the bag was simulated for a period of two days storage time by using an enzyme kinetic respiration model and a transition state model, as shown in Figures 2 and 3 respectively. It should be noted here that the accuracy of simulation results were validated by comparing the results with the experimental data measured by Makino et al. [5], and the results were in good agreement.

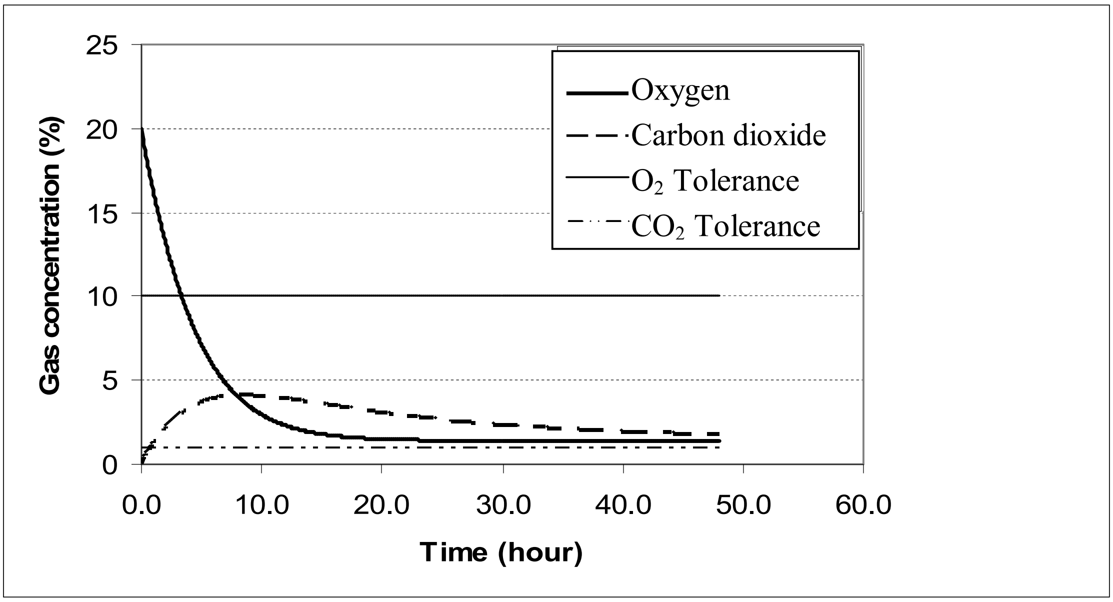


**Figure 2.** Simulation of change of gas composition inside Orega® bag of broccoli by "MAP DESIGN" under the mode of enzyme kinetic respiration model

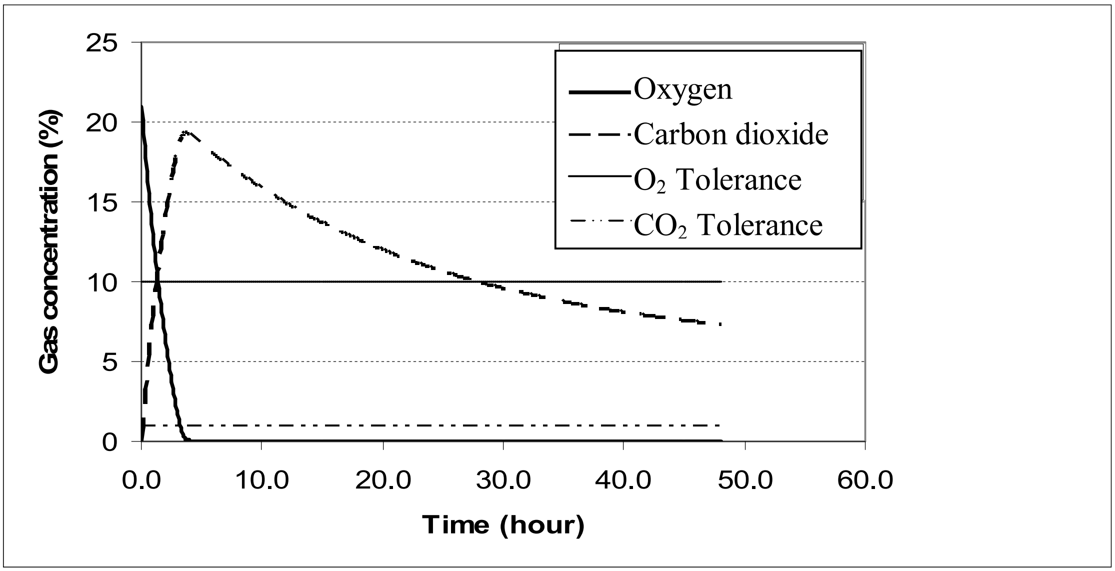


**Figure 3.** Simulation of change of gas composition inside Orega® bag of broccoli by "MAP DESIGN" under the mode of transition state respiration model

In the case of the enzyme kinetic model, Figure 2 shows that it would take about 4 hours for the $O_2$ to drop below a generally recommended tolerance limit of 10% in order to prevent the start of anaerobic respiration mode. A much faster time, only 2.8 hours, was determined for the case of the transition state model. Nevertheless, a depletion pattern of $O_2$ for both cases seemed to be in a similar fashion. However, an increment of $CO_2$ concentration inside the bag was totally different between the two models. An overshooting pattern of $CO_2$ at the beginning period of storage time was found for the transition state respiration model while a gradually increasing pattern was indicated for the enzyme kinetic model. Once the level of $CO_2$ reached the maximum value, when the $O_2$ concentration inside the bag approached zero, the level of $CO_2$ started to decrease. At that particular time, a simulation indicated that the permeation rate of $CO_2$ out of the bag was higher than the rate of creation of $CO_2$ by respiration.

An overshooting pattern of $CO_2$ concentration was related directly to the respiration quotient (Eq. 4) which was used for computing the amount of $CO_2$. Since the RQ expression is a linear function, the amount of $CO_2$ was then increased following the rapid decrease of $O_2$ obtained by the transition state model. In the case of enzyme kinetic model, the overshooting pattern disappeared since the catabolic creation of $CO_2$ was derived from the uncompetitive inhibitory mode of enzyme kinetic reaction as appearing in the form of Eq. 2. Even though the enzyme kinetic respiration model seemed to provide a much smoother profile, the result did not imply an accuracy of the model for all kinds of produce. So far, there has not been enough evidence that shows that the uncompetitive mode of enzyme kinetic model is a unique one for the produce. Instead, there are reports of other mathematical models that fit the actual respiration rate of many kinds of produce, e.g. the linear function, the exponential function, the polynomial function, and other modes of enzyme kinetic rate [10]. At the same time, nor were there any reports on the transition state model that argues for its accuracy and generality. Even so, both forms of respiration model, which were included in the MAP DESIGN, are widely used and accepted by plant scientists.

Since there has been evidence of the dependency of the respiration model on the prediction of the gas composition, estimation of product shelf life must be done with caution if the tolerance level of $O_2$ and $CO_2$ are used as indicators. It was obvious from the simulation results that the generality of the existing respiration models was not up to the point that the packaging designer needs. The dilemma of finding the best model indeed requires further research on modeling the plant respiration rate. Nevertheless, a good selection of current respiration rate models can still be helpful for designing the package. The optimization of packaging dimension by "MAP DESIGN" is discussed in the next section.

### *Optimization of packaging dimension*

The shelf life of produce packed in the package of modified atmosphere can be extended if the MAP system is designed correctly to satisfy the need of ambient conditions for a particular type of produce. The equilibrated modified atmosphere inside the package is varied based on the principle of steady-state gas and energy balance. The choice of packaging material and dimension is actually the main device for controlling an optimum atmosphere. In practice, the designing procedure must be done by trial and error until the perfect choice is found and the process requires tremendous computation time even for packaging engineers. With the "MAP DESIGN" software, all designing factors, namely packaging material and dimension, initial gas composition, and storage temperature and humidity, can be easily modified and the shelf life of the product can be rapidly predicted.

Here, only the effect of packaging dimension is demonstrated for broccoli samples. The simulation was carried out using the mass of produce and other conditions as given in the previous section, except for packaging area and volume. Once the ratio of surface area and volume of the package was set at a constant value, the effect of packaging dimension on the time to reach a steady-state gas transfer for the enzyme kinetic model could be determined as summarized in Table 1. The simulation results revealed that the steady-state gas transfer was reached after 40 hours for almost every package size unless it was very large. For this particular packaging film, a package with larger surface area retains more amount of $O_2$ while it has little effect on the level of $CO_2$. However, even for a fivefold increase of surface area (an unrealistic bag), the concentration of $O_2$ is still lower than the recommended tolerance level of 10%. When bags with smaller surface area were used for packing an equal mass of broccoli, the gas composition at steady-state was worse than that for the reference surface area of 0.069 $m^2$. The results suggest that Orega$^{®}$ film was not a good choice for broccoli packaging and other materials included in the database should be tested to check for their suitability.

**Table 1.** Effect of packaging dimension on steady-state conditions for broccoli in Orega$^{®}$ bag (using enzyme kinetic respiration model)

| Surface area of package ($m^2$) | Modification factor (%) | Time to reach steady-state (hour) | $CO_2$ (mole%) | $O_2$ (mole%) |
|---|---|---|---|---|
| 0.069 | 0 | 40 | 2.17 | 1.40 |
| 0.12 | 73.91 | 41.7 | 1.95 | 2.38 |
| 0.3 | 335 | 48 | 1.74 | 5.83 |
| 0.015 | -78.26 | 41.6 | 1.93 | 0.31 |
| 0.03 | -56.52 | 41.7 | 1.93 | 0.62 |

## Conclusions

An overview of the "MAP DESIGN" software, computational codes for the designing of MAP of fresh vegetables or fruits, was demonstrated. Simulation of a changing rate of gas composition inside the MAP under various control parameters, namely initial gas composition, temperature, humidity, and packaging material, could be easily accomplished. The capability of "MAP DESIGN" codes in tracking the gas composition revealed a substantial effect of produce respiration models on the predicted values. Shelf life determination for a similar type of product, predicted by various respiration models, may be much different. Controversially, the shelf life can be determined since the data of all respiration models were claimed for their accuracy based on independently good measurements. Therefore, the influence of the respiration models on the shelf life determination suggests that a methodology to synchronize all respiration models is needed. Nevertheless, the "MAP DESIGN" software is a set of highly efficient computation codes for the designing of the modified atmosphere package for fresh produce as long as the users provide the correct set of required factors to the codes.

## Acknowledgement

The author would like to express great appreciation for the research funding provided by Suranaree University of Technology.

## References

1. D. S. Lee, P. E. Haggar, and K. L. Yam, "Model for fresh produce respiration in modified atmosphere based on principles of enzyme kinetics", *J. Food Sci.*, **1991**, *56*, 1580-1585.
2. Y. Song, N. Vorsa, and K. L. Yam, "Modeling respiration-transpiration in a modified atmosphere packaging system containing blueberry", *J. Food Eng.*, **2002**, *53*, 103-109.
3. Y. Makino, K. Iwasaki, and T. Hirata, "Application of transition state theory in model development for temperature dependence of respiration of fresh produce", *J. Agric. Eng. Res.*, **1997**, *67*, 47-59.
4. W. Lertsiriyothin and N. Jarussinwichai, "Computational Software for the Designing of Modified Atmosphere Packaging Used for Fresh or Precut Vegetables and Fruits )'M.A.P. Design'(", Licensing No. 121623**, 2005,** Department of Intellectual Property, Ministry of Commerce, Bangkok.
5. Y. Makino, K. Iwasaki, and T. Hirata, "A theoretical model for oxygen consumption in fresh produce under an atmosphere with carbon dioxide", *J. Agric. Eng. Res.*, **1996**, *65*, 193-203.
6. Y. Makino and T. Hirata, "Modified atmosphere packaging of fresh produce with a biodegradable laminate of chitosane-cellulose and polycaprolactone", *Postharv. Bio. Technol.*, **1997**, *10* ,247-254.
7. A. A. Kader, "Respiration of gas exchange in vegetables", in "Post Harvest Physiology of Vegetables" (Ed. J. Weichmann), Marcel Dekker, New York, **1987**, Ch. 3.
8. K. L. Yam, and D. S. Lee, "Design of modified atmosphere packaging for fresh produce", in "Active Food Packaging" (Ed. M. L. Rooney), Chapman & Hall, Glasgow, **1995**, pp.55-72.
9. W. Lertsiriyothin, "Computational software for the designing of modified atmosphere packaging used for fresh or precut vegetables and fruits", Proceedings of the 8th Agro-Industrial Conference: Food Innovation, Bitec Bangna, Bangkok, Thailand,15-16 June **2006**.
10. S. C. Fonseca, F. A. R. Oliveira, and J. K. Brecht, "Modelling respiration rate of fresh fruits and vegetables for modified atmosphere packages: a review", *J. Food Eng.*, **2002**, *52*, 99-119.