Online ISSN : 2249 - 4626
Print ISSN : 0975 - 5896

Global Journal of Science Frontier Research : A Physics and Space Science

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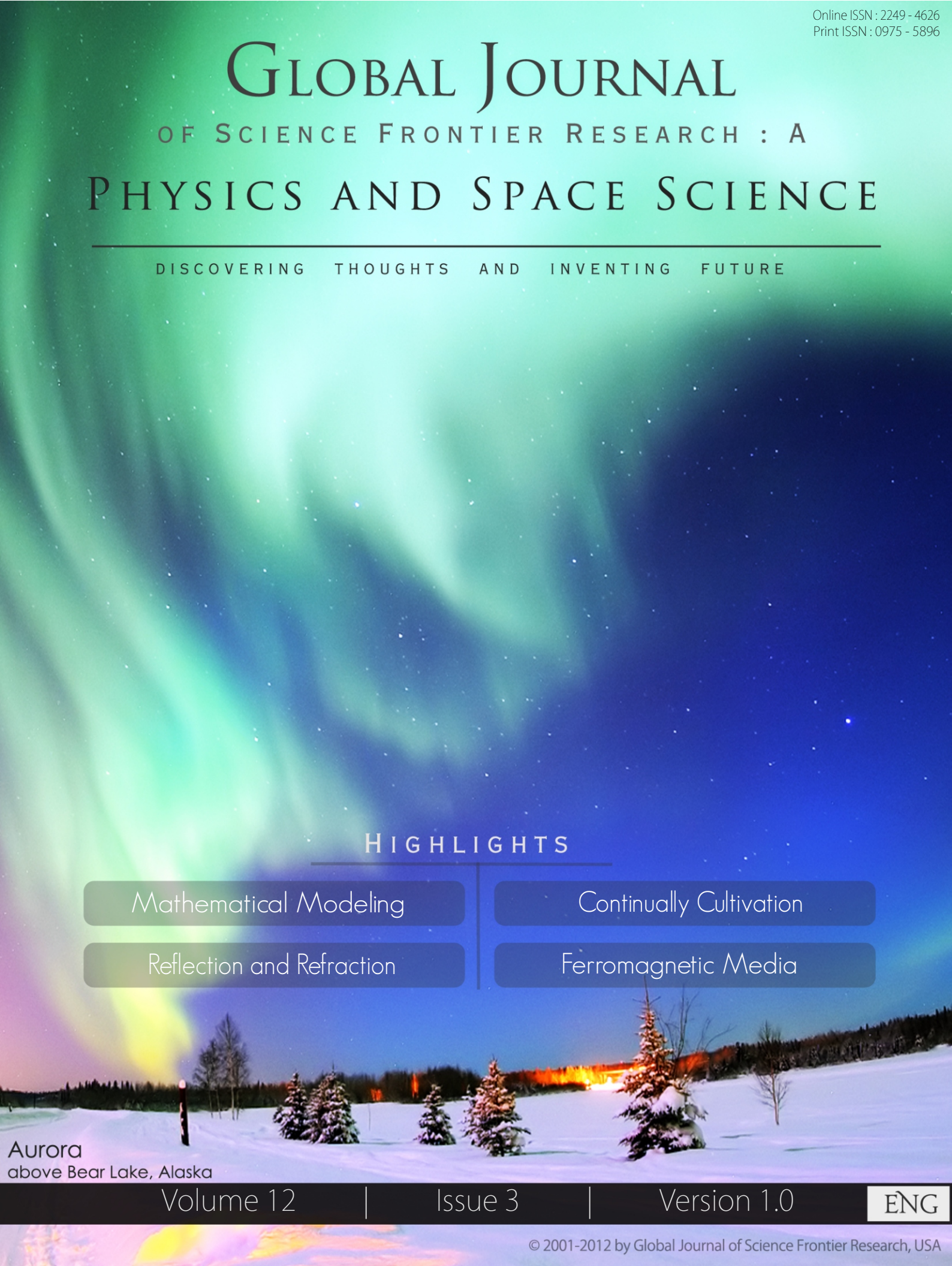

Highlights

- Mathematical Modeling
- Continually Cultivation
- Reflection and Refraction
- Ferromagnetic Media

Aurora
above Bear Lake, Alaska

Volume 12 | Issue 3 | Version 1.0 ENG

Global Journal of Science Frontier Research: A
Physics & Space Science

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Physics & Space Science
Volume 12 Issue 3 (Ver. 1.0)

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Contents of the Volume

Global Journal of Science Frontier Research
Physics & Space Science
Volume 12 Issue 3 Version 1.0 April 2012
Type : Double Blind Peer Reviewed International Research Journal
Publisher: Global Journals Inc. (USA)
Online ISSN: 2249-4626 & Print ISSN: 0975-5896

Case Study in Combining Physical and Computer Experiments

By T. Burr & Michael S. Hamada

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Abstract - Estimation of computer model parameters using field data is sometimes attempted while simultaneously allowing for model bias. One paper reports that simultaneous estimation of a bias vector and a scalar calibration parameter, which results in a "calibrated computer model," can be sensitive to assumptions made prior to data collection. Other papers show that "calibrated computer models" can lead to improved response prediction, as measured by the root mean squared prediction error (RMSE). This paper uses a simulated case study to show that the RMSE from a purely empirical prediction option (local kernel smoothing) can be smaller than the RMSE from a "calibrated computer model" option. Therefore, although we endorse "calibrated computer models," we point out that purely empirical models can provide competitive predictions in some cases.

GJSFR-A Classification: FOR Code: 029999

Strictly as per the compliance and regulations of :

Case Study in Combining Physical and Computer Experiments

T. Burr [α] & Michael S. Hamada [σ]

Abstract - Estimation of computer model parameters using field data is sometimes attempted while simultaneously allowing for model bias. One paper reports that simultaneous estimation of a bias vector and a scalar calibration parameter, which results in a "calibrated computer model," can be sensitive to assumptions made prior to data collection. Other papers show that "calibrated computer models" can lead to improved response prediction, as measured by the root mean squared prediction error (RMSE). This paper uses a simulated case study to show that the RMSE from a purely empirical prediction option (local kernel smoothing) can be smaller than the RMSE from a "calibrated computer model" option. Therefore, although we endorse "calibrated computer models," we point out that purely empirical models can provide competitive predictions in some cases.

I. Introduction

Computer models (CM) are often used to evaluate potential measurement systems. For example, a simple chemical reaction observed over time allows us to estimate a reaction rate parameter in a very simple "computer model" in Section 3 below. Even the most elaborate model is a simplification of a complex system so a key question is whether a particular CM is sufficiently accurate to adequately predict system performance. In our Section 3 example, 1.5 units remain unreacted in the real experiment, which is a feature of the true system that is not captured by the simple model.

Model bias can be an important component of CM uncertainty. Allowing for model bias while simultaneously calibrating computer model parameters has been shown to reduce the RMSE when predicting a response (Higdon et al., 2008; Unal et al., 2011; Vanli et al., 2010). Two related issues are examined in Burr and Hamada (2012): (1) to what extent does simultaneous calibration and bias fitting lead to "better" model parameter estimation, and (2) to what extent does the choice of basis functions for the bias fitting impact parameter estimates. Burr and Hamada (2012) show that simultaneous estimation of computer model parameters and model bias does not necessarily improve model parameter estimation, and that standard model choice methods such as the Bayesian information criterion cannot always reliably indicate the best basis functions or the number of basis functions.

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This paper examines whether simultaneous CM calibration and bias estimation leads to better response prediction, where response prediction is measured in one of the most common ways, using the root mean squared prediction error (RMSE).

The following sections include background for CMs and measurement system error modeling, one example, and discussion.

II. Model Validation in The Presence of Model Bias

We assume the true value of a response $y^T(x)$ is modeled with a model value $y^M(x,\theta)$ and that the model has a bias term $b_\theta(x)$ satisfying

$$y^T(x) = y^M(x,\theta) + b_\theta(x). \qquad (1)$$

The model parameters are divided into a "user-controlled" group x and calibration parameters θ following Bayarri et al. (2007), Higdon et al. (2008), and Wang et al. (2009). Examples of user-controlled parameters are physical dimensions of a nuclear measurements experimental setup that might include radiation source terms, attenuation terms, and detection system (including geometry) properties. Calibration parameters often include fundamental constants such as nuclear cross sections that define nuclear interaction probabilities. Such cross sections are often well measured but still have non-negligible measurement error in some contexts such as in estimating the neutron multiplication coefficient (Kawano et al., 2006).

Also assume the field (measured) data varies around $y^T(x)$ with random errors R satisfying

$$y^F(x) = y^T(x,\theta) + R. \qquad (2)$$

In practice, any bias in the measurement method will be confounded with model bias so to avoid indeterminacy, assume the measurement R errors have mean 0 (zero bias) and variance σ_R^2.

Equations (1) and (2) capture the notion that comparisons of measurement data to model predictions can be used to estimate model bias $b_\theta(x)$ and simultaneously to find good values of calibration parameters θ. Code accuracy is defined by the magnitude of $b_\theta(x)$. After comparing model

predictions to measured values, bias-adjustment together with estimation of θ ("calibration") can lead to more accurate predictions at new x values. These more accurate predictions should have higher accuracy as a result of such bias-adjustment and calibration.

Another goal for code validation is to predict accuracy prior to data collection by using "similar" problems that have been "validated." That is, a truly predictive science requires predicting $b_\theta(x)$ prior to observing new data, by appealing to an archived collection of "similar" problems, which is beyond our scope here (Oden et al., 2010). Our scope is to use field data and corresponding code output at various values of θ as in Eqs. (1) and (2) to simultaneously estimate $b_\theta(x)$ and θ. Burr and Hamada (2012) assessed whether the estimate $\hat{\theta}$ of θ has smaller RMSE than an estimate of θ that does not simultaneously estimate $b_\theta(x)$. Wang et al. (2009) took a somewhat different view and interpreted model validation as meaning that confidence bands around the estimate of $b_\theta(x)$ provide high confidence that a pre-specified tolerance threshold (the maximum allowable model bias) is not exceeded.

Our goal here is to assess whether the estimate $\hat{y}$ of y that arises from simultaneously estimating $b_\theta(x)$ and θ has smaller RMSE than an estimate of y that does not simultaneously estimate $b_\theta(x)$ and θ.

III. Example : Simulated Data from the Model

$$y(t) = 3.5\ \exp(-1.7t) + 1.5 + R(t)$$

A simple example with a nonlinear regression model substituting for a CM is given in Bayarri et al. (2007). Consider a nonlinear regression model $y(t) = \mu(t) + R(t)$, where $\mu(t)$ is the mean and $R(t)$ is the error at time t. Let the hypothesized (and wrong) "computer" model for $\mu(t)$ be $\mu(t) = 5\ \exp(-\theta t)$ with θ unknown. This models a chemical reaction process with initial chemical concentration 5 and reaction rate θ, both in arbitrary units, so $5\ \exp(-\theta t)$ is a standard model for the amount of chemical remaining at time t and $y(t)$ are the measured values, measured with measurement errors $R(t)$.

Let the *true model* be

$$y(t) = 3.5\ \exp(-1.7t) + 1.5 + R(t), \qquad (3)$$

Which captures the fact that 1.5 units remain unreacted in the real experiment. Figure 1 plots data simulated from this model for values of t equally spaced from 0.11 to 3.01 with residual variance $\sigma_R^2 = 0.3^2$ and fits from several models to be described. The estimated θ is $\hat{\theta} = 0.62$ with an estimated error variance $\hat{\sigma}_R^2 = 0.31$ and the solid line is the fitted values $5\ \exp(-0.62t)$. *Notice the tendency for the estimate* $\hat{\theta}$ *to be wrong in a way to attempt to compensate for the model bias. Notice however that the fit still exhibits a bias* and that $\hat{\sigma}_R^2 = 0.31$ is much larger than the true value $0.3^2 = 0.09$. The bias is also evident in the bottom plot, which plots the residuals and a linear fit to the residuals. All simulations and analyses are performed in R (R Core Development Team, 2004). For example, $\hat{\theta}$ was estimated using nls to implement nonlinear constrained least squares using the function call nls (yvals~5*exp(θ*tvals), data=dataframe1, start= list (a=1)) in R where the data (3 reps at each of 10 time values) is in the data frame named dataframe1.

Now allow for the bias $b(\theta,t)$ as in Eq. (1) and *fit the wrong model*

$$y(t) = 5\ \exp(-1.7t) + b(\theta,t) + R(t) \qquad (4)$$

to estimate θ and σ_R^2 assuming $\mu(t) = 5\ \exp(-\theta t)$. The bias $b(\theta,t)$ was fit in this example by using nls (yvals ~ 5*exp (-a*tvals) + s(tvals), data=dataframe1, start= list(θ =1)) which allows for a smooth bias term by using the default spline fit available in nls via s(tvals). Alternatively, in the 6-step procedure below, user-supplied basis functions to fit $b(\theta,t)$ are described.

When fitting $b(\theta,t)$ as just described, in 1000 simulations the average $\hat{\theta}$ is 1.69 which is within the replication error associated with 1000 simulations of the true value (1.70). However, the average (over 1000 simulations) estimated σ_R^2 is 0.64, which is considerably larger than the true value of $0.3^2 = 0.09$. Also, Figure 2 (top plot) shows that a bias adjustment to the fitted value does not adequately remove the bias. Similarly, the bottom plot of Figure 2 shows that the estimated bias $b(\theta,t)$ does not estimate the true bias very well.

Although Bayarri et al. (2007) use a prior distribution for model parameters including the bias function $b(\theta,t)$ and also report good performance of $\hat{\theta}$, it appears to be difficult to simultaneously find good estimates of $b(\theta,t)$ and θ. In fact, Bayarri et al. (2007) state and we concur that in general one cannot expect to always get good estimates of true model parameters such as θ using a "wrong" model and a bias adjustment. For example, if the coefficient of 5 in the fitted model $y(t) = 5\ \exp(-\theta t) + b(\theta,t) + \varepsilon(t)$ where $\theta = 1.7$ is changed to $\theta = 2.5$, then the average of $\hat{\theta}$ is 2.5 in 1000 simulations. Also, if the true coefficient is changed from 5 to 4.1 and the true constant is changed from 1.5 to 0.5, then the average of $\hat{\theta}$ is 3.03 in the model *with* $b(\theta,t)$ and the average of $\hat{\theta}$ is 1.69 (very close to the true value) in the model *without* $b(\theta,t)$. Because all models are "wrong" in the sense that they

are an intentional simplification of a complex reality, such findings call into question whether it is generally possible to find estimates of $b(\theta,t)$ and θ that are simultaneously close to their true values.

So it appears that the numerical example presented in Bayarri et al. (2007) is a case of getting lucky regarding estimation of θ when a bias term $b(\theta,t)$ is accommodated. Although estimation of fundamental constants θ in Eq. (1) is sometimes a goal for CMs and associated experiments, adding a bias term does not always improve estimation of θ, as this example illustrates. Nevertheless, adding the bias adjustment essentially combines a reasonable physical model (the CM or in this example an exponential term with a wrong coefficient) with a reasonable empirical model (the fitted bias). Combining two models is likely to improve interpolation and possibly extrapolation in selected circumstances outside the range of the inputs used to calibrate the model. For example, the experimenter could probably reliably create other initial concentrations and use a calibrated (but wrong) model to estimate how the initial concentration will change with time. Interpolation and extrapolation are common goals for CM.

This example can also illustrate Bayesian modeling, which is heavily used in CM evaluation. First, the model parameter θ in $\mu(t) = 5\ \exp(-\theta t)$ is known to be nonnegative and possibly also less than some reasonable upper limit. Such constraints are easily handled by using a prior probability distribution for θ that puts all of its probability on positive values, perhaps favoring a particular range of values. Second, the bias function $b(\theta,t)$ can be constrained to be a smoothly varying function of t or not. One effective way to impose a smoothness constraint is to assume that $b(\theta,t)$ is well-modeled by a Gaussian process, which typically forces $b(\theta,t)$ to be smooth by assuming nearby t values have highly positively correlated (very similar) $b(\theta,t)$ values. By varying prior assumptions regarding $b(\theta,t)$, it is possible to also model nonsmooth functions $b(\theta,t)$. However, more field data is required to model nonsmooth functions. In most applications, CM output is a "black box," with unknown functional form, so Bayarri et al. (2007) and Higdon et al. (2008) describe using basis functions to fit the response/output from CM evaluations at multiple input settings. The bias term $b_\theta(x)$ can also be fit using basis functions.

a) Simultaneous estimation of CM parameters and model bias

Following Bayarri et al. (2007) and Myers et al. (2008), we use principal components (PCs) as a basis for the CM output and Gaussian kernels as a basis for $b_\theta(x)$, and reanalyze the example. The inference steps are:

1) Evaluate the model output $y^M(x,\theta)$ at N values of θ. In the example, x is time (one dimensional) and θ is the reaction rate (a scalar).
2) Usethe values $y^M(x,\theta_1), y^M(x,\theta_2),..., y^M(x,\theta_N)$ to calculate PCs, denoted PC_Y. Mean-centering and scaling prior to PC calculation is always an option. Fit each $y^M(x,\theta_i)$ to PC_Y to choose a good dimension (usually 2 or 3 PCs are required for a good fit). In the example, $y^M(t,\theta) = 5\exp(-\theta t)$ so time t is used as the predictor which is often denoted as x, depending on context. Use a range of θ values that is broad enough for $y^M(x,\theta_1), y^M(x,\theta_2),..., y^M(x,\theta_N)$ to span the observed $y^F(x)$ values.
3) Choose a basis Z_B to fit the bias term. We used 10 equally-spaced Gaussian kernels across the range of x (t in the example), and then used the Bayesian information criterion (BIC, see below) to select a subset of 2 to 7 from the 10 available kernels.
4) Fit the experimental data $y^F(x)$ simultaneously to PC_Y and Z_B. In the example, there are three repeats for each value of t, so the error variance σ_ε^2 should be fairly well estimated unless the prior probability density is strongly concentrated away from the true value of 0.3^2.
5) Partition the fit from (4) into fit_{PCY} due to PC_Y and fit_{ZB} due to Z_B. *Use fit_{PCY} to estimate θ.* [Note: alternatively and more simply, we could use the known functional form for the computer model, $\mu(t) = 5\ \exp(-\theta t)$, to estimate θ. But in practice, one rarely knows the functional form of the computer model.] Intuitively, if model run $y^M(x,\theta_k)$ is closest in some distance measure to fit_{PCY}, then $\hat{\theta} = \theta_k$. We implemented this intuitive approach using Euclidean or Manhattan distance (the sum of absolute values of individual component differences, see the distfunction in R), and also implemented a similar approach involving fits of θ to PC_Y.
6) The results of the fit are $\hat{\sigma}_R^2, \hat{\theta}$, fit_{ZB}, and fit_{PCY}.

To implement this Bayesian approach that follows Bayarri et al. (2007) and Higdon et al. (2008), we use Markov Chain Monte Carlo (MCMC) as implemented in the metrop function in the mcmc package for R (Geyer, 2009). All MCMC results throughout this paper were obtained using metrop. The main Bayesian feature required is to constrain coefficients of PC_Y and Z_B to reasonable values. For the coefficients of PC_Y, reasonable values are determined from the range of coefficient values in Step 2. For the coefficients of Z_B, reasonable values are determined by

requiring the fitted values to be within a range determined by the experimental data $y^F(x)$.

For this example, we fixed the CM output basis to be PC_Y as described, and fixed the $b_\theta(x)$ basis to be Z_B (Gaussian kernels spread across the range of x) as described. We then tried 0 to 7 components for PC_Y and for Z_B and evaluated whether the BIC (a well-known option for model selection, see Aitken (2010), defined as BIC= - 2log(maximum likelihood) + p log(n) where p is the number of fitted parameters and n is the sample size), appeared to be effective in the sense of choosing models that gave better estimates of $b_\theta(x)$ and of θ. Because in this example there are 3 repeated measurements at each of the 10 values of x, each method can compare its estimate of σ_ε^2 to the sample variance. We found $\hat{\theta}$ to be sensitive to both the prior probability distribution for σ_ε and sensitive to the dimension of PC_Y and Z_B. See Burr and Hamada (2012) for more detail, but briefly, in each of 100 simulations we used a gamma prior distribution with mean equal to the true value 0.3 and differing standard deviations (0.01, 0.1, 10, 100) for σ_R and two PCs to fit the CM output and 0, 1, 2, 3, or 5 Gaussian kernels to fit the model bias $b_\theta(x)$ (0 kernels means that we did not allow for model bias). The resulting $\hat{\theta}$ values (where $\hat{\theta}$ is the posterior mean as estimated from the MCMC observations) varied wildly from near 0 to near 100. Average $\hat{\theta}$ values were given in Burr and Hamada (2012).

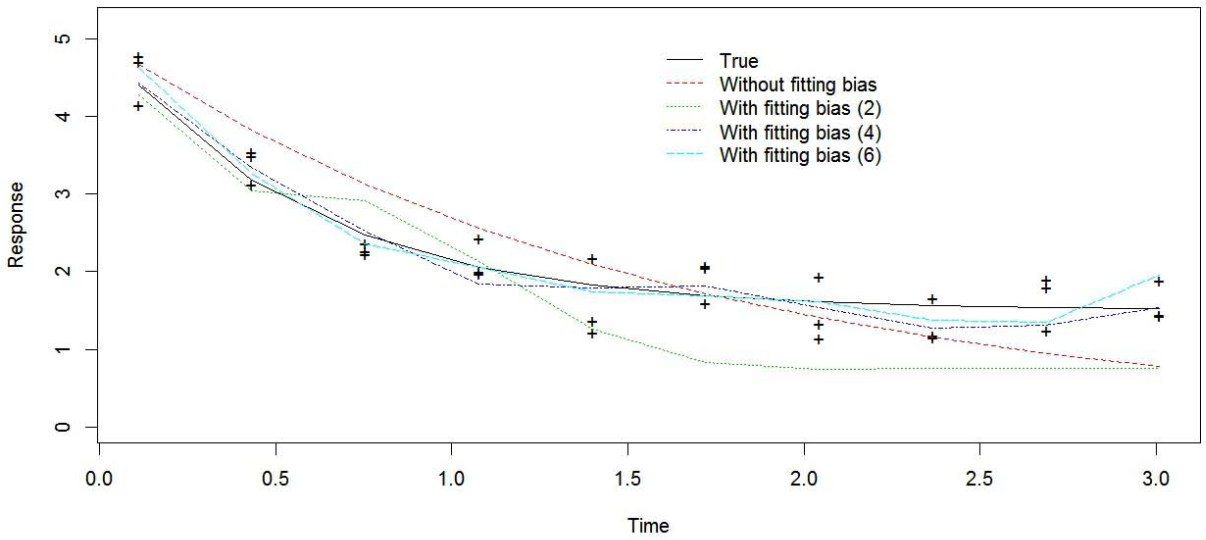

Figure 1 : Simulated data from the example using the true model $y(t) = 3.5\exp(-1.7t) + 1.5 + R(t)$ to generate data and $y(t) = 5\exp(-1.7t)$ as the CM. The predicted values without fitting a bias term and with fitting a bias term for 2, 4, or 6 basis functions are shown.

As an aside, we also used the constrained nonlinear least squares function nls as previously described, using the same type of constraints, but had convergence problems for about 20% of the realizations so we do not report nls results. In some applications however, simple application of nls is adequate for parameter estimation. Because MCMC is straight forward and easily provides posterior credible intervals for parameters, we prefer MCMC. Of course ensuring MCMC realizations have converged is time consuming, and on the basis of a several auxiliary realizations we chose proposal step sizes to get approximately a 20% acceptance rate (Geyer, 2009).

b) Root mean squared error of prediction (RMSE) in a simulation study

All RMSE results in this subsection are based on 10^4 simulations, are repeatable to ± 0.005, and $\sigma_R = 0.1$ and $\sigma_R = 0.3$ were used. The RMSE for simultaneous estimation (SE) of CM parameters and model bias and for local kernel smoothing (KS) (using lokerns) are given. The boldface entries below indicate options for which the RMSE for SE was smaller than the RMSE for KS.

First, consider predictions at the 10 times when the response is observed.

For σ_R = 0.1, the RMSE is 0.10 for SE and 0.08 for KS.
For σ_R = 0.3, the RMSE is 0.17 for SE and 0.22 for KS.

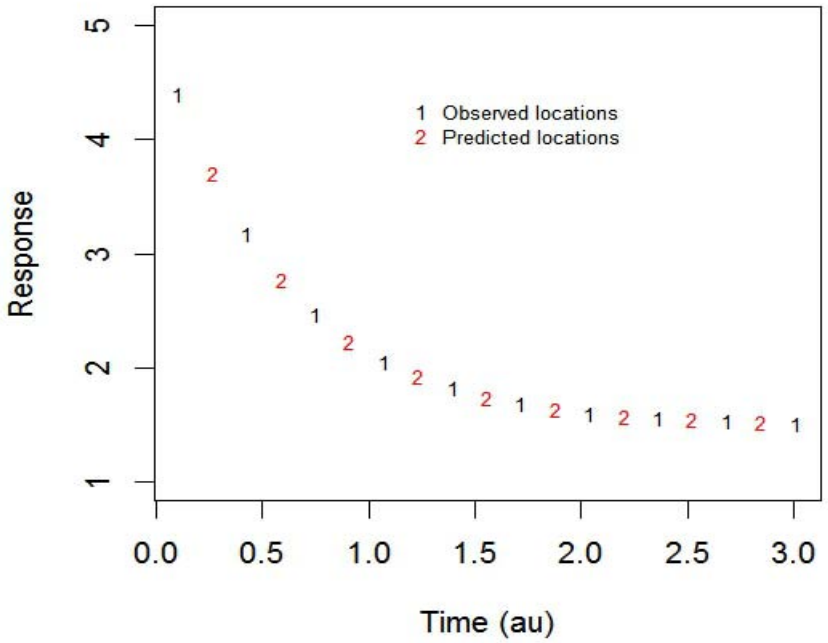

Figure 2 : The 10 times at which the response is observed, and 9 additional times where the response will also be predicted.

Next, consider predictions at the 9 new times in Figure 2, and there are several options for this type of prediction.

Option 1: Linearly interpolate the values at original 10 times to the 9 new times.

For $\sigma_R = 0.1$, the RMSE is 0.11 for SE and 0.08 for KS.
For $\sigma_R = 0.3$, the RMSE is 0.15 for SE and 0.18 for KS.

Option 2 : Linearly interpolate the basis functions from the original 10 times to the 9 new times.

For $\sigma_R = 0.1$, the RMSE is 0.11 for SE and 0.08 for KS.
For $\sigma_R = 0.3$, the RMSE is 0.15 for SE and 0.17 for KS.

Option 3 : Assume the true bias is known exactly, so exactly interpolate the true values at the original 10 times and then interpolate to the 9 new times. This option is not available in practice but serves as a basis for comparison in the unrealistic case that the true values could be known exactly at the original 10 times. The 0.03 RMSE for SE does not depend on σ_R in option 3, because the true values at the original 10 times are simply interpolated to estimate the true values at the 9 new times.

For $\sigma_R = 0.1$, the RMSE is 0.03 for SE and 0.08 for KS.
For $\sigma_R = 0.3$, the RMSE is 0.03 for SE and 0.18 for KS.

Option 4 : Similar to option 3, but use the observed data to estimate bias, so exactly interpolate the mean of the 3 observations at each of the 10 original times. This option is available in practice.

For $\sigma_R = 0.1$, the RMSE is 0.10 for SE and 0.08 for KS.
For $\sigma_R = 0.3$, the RMSE is 0.27 for SE and 0.17 for KS.

Option 5 : Use the estimate $\hat{\theta}$ of θ in the assumed known functional form $5\exp(-\hat{\theta}t)$ where $\hat{\theta}$ depends on the realization of the random noise.

For $\sigma_R = 0.1$, the RMSE is 0.80 for SE and 0.08 for KS.
For $\sigma_R = 0.3$, the RMSE is 1.56 for SE and 0.17 for KS.

Option 6 : The same as option 5, but use $= 1.7$, the true value of θ.

For $\sigma_R = 0.1$, the RMSE is 1.05 for SE and 0.08 for KS.
For $\sigma_R = 0.1$, the RMSE is 1.52 for SE and 0.17 for KS.

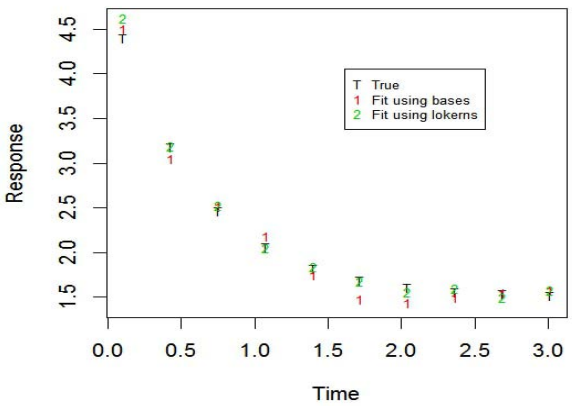

Figure 3 : The true response at each of the 10 times, and the predicted response using simultaneous estimation of CM parameters and CM bias and using local kernel smoothing, lokerns.

c) Example summary

Summary points 1-3 are found in Burr and Hamada (2012). Point 4 is the focus of this paper.

1) One can degrade performance by simulating from the same true model as assumed in the fitting, $\mu(t) = 5\exp(-\theta t)$, letting $y(t) = \mu(t) + R(t)$, and allowing for a bias term in the fit. That is, allowing for CM bias when none exists will change the inference on θ.
2) As reported in Bayarri et al. (2007), fitting a bias term does impact $\hat{\theta}$, but the bias term does not necessarily make $\hat{\theta}$ closer to θ.
3) The basis choices and the dimensions of the basis matter (for example, the value of $\hat{\theta}$ varies as the bases and dimensions of the bases change) so some sort of model selection should be considered. However, the Bayesian Information Criterion (BIC) for model selection did not perform very well. Residual diagnostics to detect patterns in residuals can be automated and appears to have more potential to guide model selection.
4) As shown above, simultaneous estimation of θ and b does not necessarily reduce the RMSE in predicting y.

Summary points 1-4 combine to suggest that simultaneous estimation of θ and b requires considerable attention to detail and careful analysis. It is is still "part art" to do a good job in simultaneous fitting of θ and b. Also, because the functional output in this example was a one-dimensional function of time, local kernel smoothing can be very competitive as a purely empirical prediction option. In higher dimensions, kernel smoothing is not as effective, although recent research suggests that nonparametric smoothing with an iterative bias correction can be effective even in high dimensions as a purely empirical smoothing and interpolation option for prediction (Cornillon et al., 2011; Burr et al., 2010 and 2011).

IV. Summary and Conclusion

Most model validation efforts include comparison of real data to corresponding code predictions. There will be iterative improvement to the models and ultimately we need apriori (prior to the next data collection) "error bars" for bias between field data and CM prediction to have defensible predictive science in this context, including in the simple reaction-rate example provided here.

Simultaneous fitting of model parameters and model bias leads to an underdetermined problem, so prior information regarding bias shape can be crucial. Even with good agreement between prior assumptions and the true state of nature, our example suggests that simultaneous estimation of model bias and model parameters does not necessarily give better estimates of model parameters nor good estimates of model bias, nor reduce the RMSE for predicting the response y. However, it can as advertized lead to better "combined model" predictions, where the combined model is the CM with fitted parameters and fitted bias. A follow-on study to investigate the effects of varying the relative sizes of error variance σ_R^2 and model bias $b(\theta, t)$ would be valuable.

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Global Journal of Science Frontier Research (A) Volume XII Issue III Version I April 2012

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Global Journal of Science Frontier Research
Physics & Space Science
Volume 12 Issue 3 Version 1.0 April 2012
Type : Double Blind Peer Reviewed International Research Journal
Publisher: Global Journals Inc. (USA)
Online ISSN: 2249-4626 & Print ISSN: 0975-5896

Basic Model of the Stationary X-ray Induced Conductivity of Wide-Gap Semiconductors

By A.O. Sofiienko, V.Ya. Degoda & V.N. Kilin
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Abstract - The concept of construction and stage-by-stage development of basic model of stationary X-ray induced conductivity for wide-gap semiconductors is proposed. Within the limits of first stage, calculation of spatial distribution of the generated electrons and holes in an ideal crystal which absorbs X-ray flux is carried out and volt-ampere characteristic is calculated.

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GJSFR-A Classification: *FOR Code: 020404*

Strictly as per the compliance and regulations of :

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A.O. Sofiienko[α], V.Ya. Degoda[σ] & V.N. Kilin[ρ]

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I. Introduction

Nowadays semiconductor detectors of X-ray and gamma radiation are the most perspective devices for realization of radioactive control in all fields of the industry, power and a science [1-4]. They have considerable advantages in comparison with scintillation and gas detectors, and also high potential of betterment in the near future. Deriving and examination of materials with wide-gap (for example, ZnSe [5, 6]; SiC [7, 8]) is perspective direction in the physics of semiconductors which have characteristics of dielectrics (due to $E_{gap} > 2.5$ eV). Under condition of moderate values of an impurity concentration and flaws of a crystalline lattice such materials can be used effectively for the solution of problems of radioactive control in extreme requirements at high temperatures and considerable dose rate [6]. For use wide-gap semiconductors as detectors of ionizing radiation with low intrinsic conductivity becomes actual developing a model of stationary X-ray induced conductivity of wide-band semiconductors which will allow to obtain such integral characteristics, as efficiency of gathering of a charge, volt-ampere and lux-ampere dependences. The X-rays that does not lead to formation of structural flaws in a crystal material even at the considerable levels of excitation have been considered as a base case.

II. Model for a Kinetics of X-ray Induced Conductivity in Wide-gap Semiconductors

First of all, the kinetic model of X-ray conductivity at first needs complete examination of a kinetics of movement of the generated free charge carriers when only one X - ray quant absorb in the semiconductor. Consideration of an ideal crystal is a convenient method of constructing the basic mathematical model for X-ray induced conductivity. Its subsequent complication associated with the introduction of components in the charge-transfer equation that describe the localization and recombination of electrons and holes in traps and recombination centers. Such an analysis has been conducted in several works [9, 10] and allowed to determine the influence of main characteristics of the material on the kinetics of charge collection in the crystal and on the value of X-ray induced conductivity. Studies have shown that for correct calculation of the kinetics of charge collection in the crystal, firstly, it is necessary to calculate spatial distribution of electrons and holes ($N^{\pm}(x,y,z,t)$) whose motion is determined by the diffusion and drift in an external electric field:

$$N^{\pm}(x,y,z,t) = \frac{N_0}{4\pi D^{\pm} t} \cdot exp\left(-\frac{(y-y_0)^2 + (z-z_0)^2}{4D^{\pm}t} \pm \frac{\mu^{\pm} E_0 \cdot (x-x_0)}{2D^{\pm}} - \right.$$
$$\left. -\frac{(\mu^{\pm} E_0)^2 t}{4D^{\pm}} \right) \cdot \frac{2}{d} \sum_{n=1}^{\infty} \left(exp\left[-\left(\frac{\pi n}{d}\right)^2 D^{\pm} t \right] sin\left(\frac{\pi n x}{d}\right) sin\left(\frac{\pi n x_0}{d}\right) \right), \quad (1)$$

where N_0 - an amount of the generated electrons and holes after absorption of X-ray quantum, x_0 - coordinate of absorption of a X-ray quantum in the semiconductor, d - distance between electrodes on crystal, E_0 - intensity of an external electric field, $D^{\pm}$ - diffusion constants of charge carriers, $\mu^{\pm}$ - mobilities of charge carriers. While considering the absorption of one X-ray photon another important conclusion can be made: the value of the intrinsic electric field generated electron and hole, which quickly relaxes during 0.1-1 ns.[9], is small. This means that during the drift of electrons and holes at low excitation levels Coulomb interaction between them can be neglected. However, in many practical problems it is important to measure not only separate impulses of a current in a crystal which arise at absorption of separate quanta, but also measuring common a gamma- or X-ray induced conductivity. In this case it is necessary to consider the absorption in a crystal of a stream of quanta, to consider their spatial distribution, allocation of the localized charge carriers on traps, electric fields of the free and localized electrons and holes. The logic of building of a kinetics X-ray induced conductivity at absorption of one X-ray quantum can be used to develop the model

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stationary X-ray induced conductivity in wide-gap semiconductors.

Stationary X-ray induced conductivity arises during prolonged irradiation of semiconductors by the stream of quanta, when average concentrations of the generated electrons and holes reach equilibrium values. In general case it is possible to distinguish some consecutive stages in development of model stationary X-ray induced conductivity. First stage - development of a basic model of stationary X-ray induced conductivity for an ideal semiconductor, which includes the choice of the geometry of the detector, the calculation of spatial distributions of electrons and holes which drift in an external electric field, the calculation of its own electric field of electrons and holes (when levels of excitation are significant), the calculation of the stationary X-ray induced conductivity. The second stage of development of model stationary X-ray induced conductivity is an addition to model of the ideal semiconductor by traps for electrons and holes. Depending on quantity of time of drift of electrons and holes and time of localization on traps it is possible to consider traps shallow or deep. The third stage is an adding of recombination centers to model of the semiconductor with traps. Results obtained at the third stage of modeling may be compared with the results of experimental measurements of current-voltage and lux-ampere characteristics.

III. The Spatial Distribution of Concentrations of Electrons and Holes in an Ideal Semiconductor

Let's choose the following scheme of measuring stationary X-ray induced conductivity. On rectangular sample ($d \times L \times H$) directed the flow of X-rays and its direction is perpendicular to the vector of external electric field $E_0 = U_0/d$. The model of the detector and the scheme of measuring of a current of stationary X-ray induced conductivity are shown on fig. 1. In the plane OXZ at the depth y in the layer dy per second absorbed by the following number of quanta: $dF(y) = F_0 \cdot \kappa_X \cdot \exp(-\kappa_X \cdot y) \cdot dy$, where F_0 - the flux of X-rays ($\text{cm}^{-2} \cdot \text{s}^{-1}$), κ_X - the absorption coefficient of X-rays. At absorption of one X-ray quantum will create on the average $N_0 = h\nu_X / 3E_g$ the electron-hole pairs, where $h\nu_X$ – energy of X-ray quantum, E_g – band gap of the semiconductor. Immediately after the generation some electrons and holes may recombine with each other at the centers of recombination (glow), so their number is at the stage of the drift can vary by $\eta \leq 1$ times.

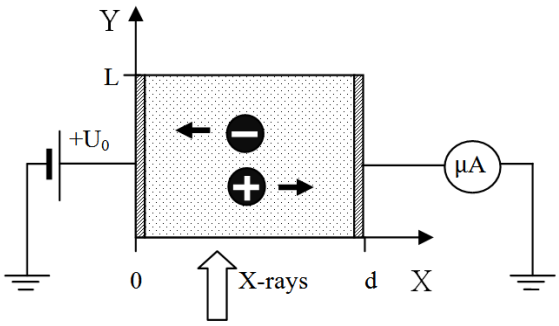

Fig.1 : Model of the detector and the scheme of measuring of a current of stationary X-ray induced conductivity (top view).

The rate of the generation of electrons and holes N_G ($\text{cm}^{-3} \cdot \text{s}^{-1}$) at a depth [y; y+dy]:

$$N_G(y) = N_{G0} \cdot e^{-\kappa_X \cdot y}, \; N_{G0} = F_0 \cdot \left(\frac{h\nu_X}{3E_g} \cdot \eta \right) \cdot \kappa_X \qquad (2)$$

The kinetics equations of motion of electrons and the holes in the ideal semiconductor:

$$\frac{\partial N^{\pm}}{\partial t} = N_G + D^{\pm} \cdot \Delta N^{\pm} \mp \mu^{\pm} \cdot \vec{\nabla}\left(\vec{E_0} \cdot N^{\pm} \right), \qquad (3)$$

And boundary conditions: $N^{\pm}(0) = N^{\pm}(d) = 0$. In the case of stationary X-ray induced conductivity $\partial N^{\pm} / \partial t = 0$. In the equations (3) the electric field which is created by electrons and holes at drift is not considered. It superimposes restriction on the peak value of rate of generation of charge carriers: $N_{G0} < 10^{14}$ $\text{cm}^{-3} \cdot \text{s}^{-1}$. The equations (3) have following approximate solutions:

$$\begin{cases} N^{-}(x,y) \approx \dfrac{N_{G0} \cdot e^{-\kappa_X \cdot y}}{\mu^{-} \cdot E_0} \cdot \left\{ d \cdot \left(\dfrac{1 - e^{-\frac{e \cdot E_0 \cdot x}{k_B \cdot T}}}{1 - e^{-\frac{e \cdot E_0 \cdot d}{k_B \cdot T}}} \right) - x \right\} \\ N^{+}(x,y) \approx \dfrac{N_{G0} \cdot e^{-\kappa_X \cdot y}}{\mu^{+} \cdot E_0} \cdot \left\{ x - d \cdot \left(\dfrac{e^{\frac{e \cdot E_0 \cdot x}{k_B \cdot T}} - 1}{e^{\frac{e \cdot E_0 \cdot d}{k_B \cdot T}} - 1} \right) \right\} \end{cases} \qquad (4)$$

During calculations Einstein's relation has been used: $D^{\pm} = \mu^{\pm} \cdot k_B \cdot T / e$, where k_B - a Boltzmann constant, T - crystal temperature, e – elementary electronic charge. Spatial distributions of electrons and holes essentially depend on their mobility and intensity of an exterior electric field. Result of calculation of spatial distributions of electrons and holes in ZnS are shown on fig.2. at $E_0 = 0.1$ V/cm and $E_0 = 1.0$ V/cm (for saving of one scale the electron concentration is incremented in 23 times, since $\mu^{-} / \mu^{+} \approx 23$). In the absence of an external electric field ($E_0 = 0$) the spatial distribution of electrons and holes is determined only by diffusion and recombination at the electrodes and consequently is the symmetrical. The drift current of

non-equilibrium carriers in an external electric circuit determined by the ratio Ramo-Shockley [11]:

$$i_X(U) = \frac{U}{d^2} \cdot \left(q^-(U) \cdot \mu^- + q^+(U) \cdot \mu^+ \right) \quad (5)$$

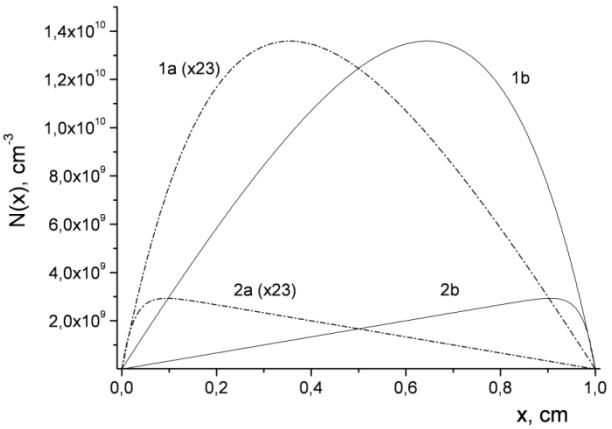

Fig.2 : Spatial distributions of electrons and holes on surface ZnSe at E_0 = 0.1 V/cm (1a – electrons, 1b - holes) and E_0 = 1 V/cm (2a – electrons, 2b - holes); y = 0, d = 1 cm, $N_{G0} = 10^{11}$ cm-3·s-1, $\mu^- = 700$ cm^2·V^{-1}·s^{-1}, $\mu^+ = 30$ cm^2·V^{-1}·s^{-1}, $k_X = 240$ cm^{-1}.

The charge of electrons and holes that create a drift current:

$$q^{\pm}(U) = e \cdot H \cdot \int_0^d \int_0^L N^{\pm}(x, y) \cdot dxdy \,, \quad (6)$$

Where H - height of crystal on axis OZ. Current of stationary X-ray induced conductivity:

$$i_X(U) = e \cdot F_0 \cdot \left(\frac{h\nu_X}{3E_g} \cdot \eta \right) \cdot d \cdot H \cdot \left(1 - \frac{2k_B \cdot T}{e \cdot U} \right) \quad (7)$$

The peak current of stationary X-ray induced conductivity in the ideal semiconductor is equal to a charge generation rate at absorption of a stream of X-ray quanta:

$$\lim_{U \to \infty} i_X(U) = e \cdot F_0 \cdot d \cdot H \cdot \left(\frac{h\nu_X}{3E_g} \cdot \eta \right) = \frac{dQ_0}{dt} \quad (8)$$

It is obvious that formula (8) can also be obtained by adding up all of the current pulses from the individual X-rays, which is true only for the ideal model of a semiconductor at low excitation levels. Thus, when the concentration of the generated electrons and holes in an ideal crystal are negligible and their electric field can be neglected, the current-voltage characteristic is described by a sublinear function, which quickly reaches saturation (at $E_0 > 10$ V/cm). It is worth to note that in (8) no longer dependence on the characteristics of the semiconductor disappears.

IV. Conclusions

The basic model of stationary X-ray induced conductivity for wide-gap semiconductors which is grounded on calculation of average spatial distributions of electrons and holes in a crystal is offered and allows to obtain such integral characteristics of the semiconductor as efficiency of collection of a charge, volt-ampere and lux-ampere characteristics at low levels of stationary excitation. The following stage of development of model is consideration of recombination centers and calculation of spatial distributions of the localized electrons and holes on the traps, calculation of their electric fields which can exceed considerably external fields at the considerable levels of excitation.

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Global Journal of Science Frontier Research (A) Volume XII Issue III Version I April 2012
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Global Journal of Science Frontier Research
Physics & Space Science
Volume 12 Issue 3 Version 1.0 April 2012
Type : Double Blind Peer Reviewed International Research Journal
Publisher: Global Journals Inc. (USA)
Online ISSN: 2249-4626 & Print ISSN: 0975-5896

Mathematical Modeling of L-Lyzin Biosynthesis Process during Continually Cultivation

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Abstract - A mathematical model with concentrated parameters of L-lyzin biosynthesis process during continually cultivation of the Brevibacterium flavum type microbial population is proposed. A parametrical identification of the model's kinetic variables is carried out. A mathematical model with distributed parameters of the same biotechnological process is developed. The stability of the stationary solutions of the obtained dissipative structure is investigated.

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I. Introduction

The presence of such a variety of mathematical models indicates the lack of a fundamental theory of growth and reproduction of biological objects. All the models known in the literature can only be applied for the description and analysis of some particular aspects of the growth and reproduction processes of a specific biological object. The attempts to be expanded the range of application of these models and their utilization at the development of a general theory, enter into a disagreement with the factual data usually. Moreover, in few of these works the qualitative theory of ordinary differential equations has been used as a method for state analysis of biological objects [1]. The phase analysis gives a good possibility every nonlinear system, described with ordinary differential equations to be studied qualitatively.

Mathematical models of the microorganisms cultivation processes in a bioreactor are developed, taking into account the kinetics of the final or intermediate metabolism products formation, the kinetics of biomass growth and the kinetics of sub-stratum consumption. All these models are based on different hypotheses about the acting biosynthesis mechanism: the presence of limiting substrata, inhibitors or activators of growth, and the degree of their impact on the velocity of the biomass and product formation [2].

Another peculiarity is applied of the empirical approach at the development of mathematical models. The limiting factors are many in number which influence on the cells growth. Because of that in every specific case the biomass growth velocity depending on the limiting factor concentrations is determined experimentally. In the kinetics of the "exact" microbiological systems it is assumed that the bioreactor sizes are small, and the mixing leads to an instant leveling of the concentrations of all substances into the whole volume of the bioreactor. Taking into consideration the above limits the mathematical models are obtained, which are not adequate to the actual processes. In these models it is assumed that the cultural medium of the bioreactor is homogeneous (all concentrations of biologically important substances are an even distributed). Thus, for the more precisely description of the biosynthesis processes in the bioreactor, it is necessary the diffusion processes to be reflected in the mathematical models. As a result all concentrations will be considered as functions of the time and space coordinates. The accounting of all these circumstances gives a possibility to be developed a more adequate model to the actual process. In order to solve such a problem, it is necessary to be used the qualitative theory of distributed kinetic systems.

II. Mathematical Model with Concentrated Parameters of L Lyzin Biosynthesis Process During Continually Cultivation of The Brevibacterium Flavum Type Microbial Population

The mathematical model of the L-lyzin biosynthesis process during continually cultivation of the *Brevibacterium flavum* type microbial population is obtained as a variant of the Ohno *et al.* model [3]. This model reflects the material balance of the basic components of the cultural medium and has the following form:

$$\frac{dX}{dt} = \mu_m \frac{S}{K_S + S} X - DX,$$

$$\frac{dS}{dt} = -\frac{\mu_m}{Y_{X,S}} \frac{S}{K_S + S} X + D(S^0 - S),$$

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$$\frac{dL}{dt} = Y_{L,X}\frac{dX}{dt} - DL, \quad (1)$$

where:

X – biomass concentration $[g/1]$;

S – sugar concentration $[g/1]$;

L – lyzin concentration $[g/1]$;

μ_m – maximum relative velocity of the biomass growth $[s^{-1}]$;

$Y_{X,S}$ = dX / dS-stoichiometry of the biomass to the sugar [–];

$Y_{L,X}$ – constant [–];

$K_S = k_{x,s} / r_{x,s}$, where $r_{x,s}$ is the velocity of the transformation of the biomass and sugar in biomass-sugar complex (XS), and $k_{x,s}$ is the velocity of the transformation of the biomass-sugar complex in biomass and sugar $[g/l]$ [4].

D – diluting velocity) $[s^{-1}]$;

S^0 – sugar concentration in the feeding medium $[g/1]$.

It is supposed that an ideal mixing is carried out in the bioreactor and all the parameters of the model are constants during the biotechnological process. As a result the proposed model (1) can be examined as a nonlinear autonomous system of ordinary differential equations with concentrated parameters.

Depending on the microorganisms cultivation technology for the specific process of L-lyzin biosynthesis nine replicable experiments were carried out under identical conditions in a bioreactor with volume 10 m^3. The experimental data of the biomass (X), sugar (S) and lyzin (L) concentrations are obtained under laboratory conditions by means of samples taken every four hours from the cultural medium of the bioreactor. The processing of these experimental data is accomplished by using of the fuzzy sets apparatus [5]. The smoothed experimental values for X, S and L at the different periods of time are shown in Table 1 and marked by "E ".

For this biotechnological process is speciality that the microorganisms nutrition with substratum (sugar) in the bioreactor is carried out at constant diluting velocity ($D = 0.025\ s^{-1}$). The sugar concentration in the feeding medium ($S^0 = 19\ g/1$) is also constant and equal to the initial sugar concentration in the bioreactor (S_0).

The numeric values of the parameters in system (1) μ_m, K_S, $Y_{X,S}$, $Y_{L,X}$ can be found by minimizing of the following functional:

$$J = \sum_{j=1}^{10}[(X_j^E - X_j^T)^2 + (S_j^E - S_j^T)^2 + (L_j^E - L_j^T)^2], \quad (2)$$

Where: $F_j^E = \{X_j^E, S_j^E, L_j^E\}$ is a vector of the smoothed experimental values of the biomass, sugar and lyzin concentrations at the j-th period of time (Table 1);

$F_j^T = \{X_j^T, S_j^T, L_j^T\}$ is a vector of the theoretically obtained values of the biomass, sugar and lyzin concentrations at the j - th period of time by solving of the system of ordinary differential equations (1).

Table. 1 : Obtained experimental "E" and theoretical "T"' values of the biomass, sugar, and lyzin concentrations at the different moments of time.

Time [h]	X^E [g/1]	X^T [g/1]	S^E [g/1]	S^T [g/1]	L^E [g/1]	L^T [g/1]
0	3.0	3.00	19.0	19.00	0.0	0.00
4	5.1	5.28	15.2	15.56	5.6	5.56
8	9.5	8.76	9.4	10.53	14.1	13.68
12	13.1	12.80	4.1	4.78	22.3	22.95
16	14.3	15.04	1.0	1.48	26.9	28.28
20	14.8	15.35	1.0	0.82	28.7	2936
24	15.0	15.22	1.0	0.75	29.6	29.47
28	15.1	15.07	1.0	0.75	29.9	29.47
32	15.2	14.92	1.0	0.76	30.0	29.46
36	15.2	14.79	1.0	0.76	30.1	29.45
40	15.0	14.67	1.0	0.77	30.0	29.43

System (1) can be solved by means of the Runge-Kutta method. The initial values of the parameters μ_m, K_S, $Y_{X,S}$, $Y_{L,X}$ in system (1) are determined on the basis of reference data for similar biotechnological processes, as well as taking into account the specific character of our process of the L-lyzin biosynthesis [6]. When an apriori information for the initial parameter values is lacking they are

determined randomly. In this case there exists a danger after minimizing of functional (2) such values of the parameters of the process to be obtained which are inadmissible from a physical point of view. The initial parameter values of the specific process of L-lyzin biosynthesis are presented in Table 2, line 1.

The minimum of functional (2) is found by using of an optimization method of the adaptive random search [7]. As a result of the parametrical identification, such numeric values of the parameters of the specific process of L-lyzin biosynthesis are obtained, which are physically acceptable and warrant a minimum of the root- mean-square criterion (the values of the parameters are represented in Table 2, line 2). In Table 1 the theoretical values of the biomass, sugar and lyzin concentrations at the different periods of time marked by "T" are obtained exactly for such values of the parameters whose functional (2) has a minimum.

It can be seen from Table 1 that the deviation of the smoothed experimental data from the theoretically obtained values is by a negligible margin, which suggests the conclusion that the proposed nonlinear system with concentrated parameters (1) describes the actual biotechnological process in a sufficiently accurate way.

In a qualitative aspect the phase portraits in the planes (X, S) and (L, S) are identical, since in the proposed model (1) a proportional dependence of the change of the L-lyzin concentration (L) from the change of the biomass concentration (X) exists. This circumstance gives a possibility the autonomous system (1) to be investigated in the phase plane (X, S) qualitatively by substituting of the obtained numerical values of the parameters μ_m, K_S, $Y_{X,S}$, $Y_{L,X}$ in it. (Tab. 2).

The nonlinear system (1) has two fixed points whose coordinates are:

$$1st-fixed\quad point \rightarrow X_1^{'}=0,\quad S_1^{'}=S^0=19$$

$$2nd-fixed\quad point \rightarrow X_2^{'}=\frac{-\mu_m K_S D^2+\mu_m^2 D S^0-\mu_m D^2 S^0}{\alpha D\mu_m-\alpha D^2}$$

$$S_2^{'}=\frac{K_S D}{\mu_m-D}=0.8432, \tag{3}$$

Table 2 : First Line – Parameters Initial Values, Second Line – Parameter Values Obtained at the Parametrical Identification.

No	μ_m	K_S	$Y_{X,S}$	$Y_{L,X}$
1.	0.1	1.0	1.0	1.0
2.	0.2333	7.0258	0.7439	2.1705

For every fixed point the local coordinates may be introduced by using of the formulae:

$$\xi_j=X-X_j^{'},\quad \eta_j=S-S_j^{'},\quad j=1\div 2,$$

i.e. every fixed point with coordinates $(X_j^{'}, S_j^{'})$ in the coordinate system (X, S) is transformed at the beginning of new coordinate system (ξ, η).

In (1) the differential equations' right-hand parts for X and S are expanded into a Taylor series in some neighbourhood of every fixed point $(X_j^{'}, S_j^{'})$ j = 1 ÷ 2. Passing to local coordinates system (1) is transformed into:

$$\begin{aligned}\frac{d\xi_j}{dt}&=\xi_j\frac{\partial F_1}{\partial X}\left(X_j^{'},S_j^{'}\right)+\eta_j\frac{\partial F_1}{\partial S}\left(X_j^{'},S_j^{'}\right)+R_1\left(\xi_j+X_j^{'}\eta_j+S_j^{'}\right)=F_1(\xi,\eta),\\ \frac{d\eta_j}{dt}&=\xi_j\frac{\partial F_2}{\partial X}\left(X_j^{'},S_j^{'}\right)+\eta_j\frac{\partial F_2}{\partial S}\left(X_j^{'},S_j^{'}\right)+R_2\left(\xi_j+X_j^{'}\eta_j+S_j^{'}\right)=F_2(\xi,\eta).\end{aligned} \tag{4}$$

In order to study system (4) qualitatively the linearization theorem should be taken into account. It reads: if the nonlinear system has a simple fixed point with coordinates $(0,0)$, then in the neighbourhood of this fixed point the phase portraits of the nonlinear system and its linearization are equivalent qualitatively only if the fixed point of the linearized system is not a centre [8].

The first requirement of the linearization theorem is executed since the matrices

Have simple fixed points (X'_j, S'_j) j = 1 ÷ 2 (further on this is seen from (5)).

After linearization of system (1) the only solution of the matrix equations, A_jY_j=0 is

$$Y_j = \begin{bmatrix} \xi_j \\ \eta_j \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, j = 1 \div 2$$

Thus system (1) has two simple fixed points transformed at the beginning of the coordinates of the phase plane (ξ, η). In the concrete case system (1) has the following matrices $A_j, j = 1 \div 2$:

$$A_j = \left[\begin{matrix} \frac{\partial F_1}{\partial X} & \frac{\partial F_1}{\partial S} \\ \frac{\partial F_2}{\partial X} & \frac{\partial F_2}{\partial S} \end{matrix} \right]_{(X,S)=(X'_j, S'_j), j=1\div 2,}$$

$$A_1 = \begin{bmatrix} a_1 & b_1 \\ c_1 & d_1 \end{bmatrix} = \begin{bmatrix} 0.1453 & 0.0000 \\ -0.2290 & -0.0250 \end{bmatrix}, A_2 = \begin{bmatrix} a_2 & b_2 \\ c_2 & d_2 \end{bmatrix} = \begin{bmatrix} 0.0000 & 0.3576 \\ -0.0336 & -0.5056 \end{bmatrix}. \quad (5)$$

The second requirement of the linearization theorem reads that a qualitative equivalence between the nonlinear system (1) and its linearization (4) exists only if the fixed points of the linearized system are not a centre. This requirement is executed since the matrices $A_j, j = 1 \div 2$: have different and real proper values. The fixed points can be from centre type, if the matrices Aj have complex proper values. For the nonlinear system (1) the conditions of the linearization theorem are executed, which makes possible further on at the phase analysis its linearized version (4) to be used.

After the canonization of system (4) the Jordan forms J_j of the matrices A_j are obtained in the form of:

$$J_1 = \begin{bmatrix} 0.1453 & 0.0000 \\ 0.0000 & -0.0250 \end{bmatrix}, J_2 = \begin{bmatrix} 0.0250 & 0.0000 \\ 0.0000 & -0.4806 \end{bmatrix}.$$

For the first fixed point the proper values are $\lambda_1^{(1)}$ = 0.1453 and $\lambda_2^{(1)}$ = – 0.0250 respectively. In this case the proper values have real numbers with converse signs so this fixed point generates a saddle at the beginning of the phase plane coordinates (ξ, η). For the second fixed point the proper values are negative real numbers – $\lambda_1^{(2)}$ = – 0.0250, $\lambda_2^{(2)}$ = 0.4806, and thus this fixed point generates stable node at the beginning of the phase plane coordinates (ξ, η). For the exact construction of the full phase portrait of the nonlinear system (1) it is necessary to be found the vertical (dX/dt = 0) and horizontal (dS/dt = 0) isoclinals additionally. The biomass and sugar concentrations have real positive values. As a result it is necessary to be constructed the full phase portrait of nonlinear system (1) only for the 1^{st} – quadrant of the phase plane (X, S). Passing from local coordinates (ξ, η) to real coordinates (X, S) and taking into consideration the linearization theorem.

III. Mathematical Model with Distributed Parameters of L-Lyzin Biosynthesis Process During Continually Cultivation of the Brevibacterium Flavum Type Microbial Population

At the qualitative investigation of the model with distributed parameters it is accepted that the space is one-dimensional in which the different reactions of the biosynthesis are carried out. In this special case the bioreactor is considered as long and narrow tube of which the one end is opened and through its pass substratum (sugar) with concentration ($S°$). For the model with distributed parameters it is necessary to be investigated the stability of the space similar stationary solutions (3). This investigation will be carried out taking into consideration the following limiting conditions:

$$\left.\frac{\partial X}{\partial r}\right|_{r=0} = \left.\frac{\partial X}{\partial r}\right|_{r=R}, \quad \left.\frac{\partial S}{\partial r}\right|_{r=0} = \left.\frac{\partial S}{\partial r}\right|_{r=R}, \quad (6)$$

Where r=0 and $r = R = 5\,m$ are the coordinates of the beginning and end sections of the bioreactor.

Accounting for the diffusion processes in the specific process of L-lyzin biosynthesis the model with distributed parameters has the following form:

$$\frac{dX}{dt} = \mu_m \frac{S}{K_S + S} X - DX + D_X \frac{\partial^2 X}{\partial r^2}, \quad (7)$$

$$\frac{dS}{dt} = -\frac{\mu_m}{Y_{X,S}} \frac{S}{K_S + S} X + D\left(S^0 - S\right) + D_S \frac{\partial^2 S}{\partial r^2},$$

Where D_X and D_S are coefficients of the biomass and sugar diffusions respectively.

In order to be stable the distributed system (7), it is necessary small disturbances of the forces acting upon the system to provoke small deviations

from its stationary solutions (3). The investigation of the stability is carried out on the basis of the linear distributed system analysis:

$$\frac{\partial \xi_j}{\partial t} a_j \xi_j + b_j \eta_j + D_X \frac{\partial^2 \xi_j}{\partial r^2}$$
$$\frac{\partial \eta_j}{\partial t} c_j \xi_j + d_j \eta_j + D_S \frac{\partial^2 \eta_j}{\partial r^2} \quad (8)$$

Where $\xi_j(t, r)$ and $\eta_j(t, r)$, $j = 1 \div 2$, are small deviations from the space similar solutions (X_j, S_j), and a_j, b_j, c_j, d_j, $j = 1 \div 2$, are the values of the coefficients obtained in (5).

At the limiting conditions (6) the solution of system (8) is searched in the form of:

$$\xi_j(t, r) = A_j e^{p^{(j)} t} e^{i 2\pi r/\lambda}, \quad \eta_j(t, r) = B_j e^{p^{(j)} t} e^{i 2\pi r/\lambda}, \quad (9)$$

Where A_j and B_j, $j = 1\text{-}2$, are constants.

By substituting of the solutions (9) in system (8) it is obtained:

$$\frac{d\xi_j}{dt} = \left[a_j - D_X \left(\frac{2\pi}{\lambda} \right)^2 \right] \xi_j + b_j \eta_j,$$
$$\frac{d\eta_j}{dt} = c_j \xi_j + \left[d_j - D_S \left(\frac{2\pi}{\lambda} \right)^2 \right] \eta_j, \quad (10)$$

From system (10) for the complex frequency (p) the following characteristical polynomial is obtained:

$$\left[p^{(j)} - a_j + (2\pi/\lambda)^2 D_X \right] \left[p^{(j)} - d_j + (2\pi/\lambda)^2 D_S \right] = b_j c_j, \quad (11)$$

where:

λ – wave length;

$u = (2\pi/\lambda)^2$ – wave number.

It is established experimentally that for the specific process of L-lyzin biosynthesis the diffusion coefficients have the following values: $D_X = D_S = 1$.

For the first fixed point $p^{(1)}_{1,2}$ is defined from the equality (11) by the formulae:

$$p^{(1)}_{1,2} = \frac{a_1 + d_1}{2} - (D_X + D_S)\frac{u}{2} \pm \frac{1}{2}\left[u(D_X - D_S) - (a_1 - d_1) \right],$$

where: $p_1^{(1)} = -0.0250 - u$, $p_2^{(1)} = -0.1453 - u$.

Analogous for the second fixed point $p^{(2)}_{1,2}$ has the form of:

$$p^{(2)}_{1,2} = \frac{d_2}{2} - (D_X + D_S)\frac{u}{2} \pm \frac{1}{2}\sqrt{\left[u(D_X - D_S) + d_2 \right]^2 + 4b_2 c_2},$$

where: $p_1^{(2)} = -0.4806 - u$, $p_2^{(2)} = -0.0250 - u$.

As a result the stability of system (7) at different wave lengths can be investigated by the help of the quadratic equation (11) and its solutions.

For the first fixed point the characteristical equation (11) has two real roots: $p_1^{(1)} < 0$ for all λ values, $p_2^{(1)} > 0$ for $\lambda > \lambda_2 = 16.4751$ and $u < u_2 = 0.1453$. In this case at small deviations $\xi(t, r)$ and $\eta(t, r)$ in the immediate proximity of X'_1 and S'_1 the linear distributed system have a fixed point of saddle type. The limits of wave numbers (u), at which this fixed point generates a saddle, are given with the equality:

$$u_{1,2} = \left(\frac{2\pi}{\lambda_{1,2}} \right)^2 = \frac{1}{2D_X D_S}\left[(a_1 D_S + d_1 D_X) \pm \sqrt{(a_1 D_S + d_1 D_X)^2 - 4D_X D_S (a_1 d_1 - b_1 c_1)} \right].$$

In the concrete case for $\lambda_2 = 16.4751 < \lambda \leq \infty$ and $0 \leq u < u_2 = 0.1453$ (if $\lambda_2 \to \infty$ => $u_2 = 0$) system (7) have a fixed point of saddle type, and the space periodical and independent of time solutions (dissipative structure) can arise. The stability of the stationary solution of the first fixed point has not be studied, since this fixed point can not be reached from a physical point of view. For the specific process of L-lyzin biosynthesis the biomass concentration (X) is changed from 3 to 15 [g/l], and the sugar concentration (S) – from 0.5 to 19 [g/l]. The limits of these concentrations are determined depending on the specific technology of the microorganisms cultivation.

For all λ values of the second point $p_1^{(2)} < 0$ and $p_2^{(2)} < 0$. This shows that in the immediate proximity of this fixed point (X'_2, S'_2) a stable node is generated, and at small deviations from it the stationary solution of the second fixed point for all wave length (λ) values is stable.

As a final result of the analysis two variants are possible:

a) If $\lambda > \lambda_2 = 16.4751$ then in system (7) stable or unstable space periodical and independent of time solutions (dissipative structure) can arise. This possibility is ignored since the first fixed point can not be reached from a physical point of view.
b) If $\lambda < \lambda_2 = 16.4751$ it is obviously that system (7) is stable and space periodical and independent of time solutions can not arise in it.

IV. Conclusion

In the proposed work the obtained results show that at definite conditions space periodical and independent of time solutions (dissipative structure) can arise. The carried out phase analysis gives an answer to the question for the stability of the stationary solutions of the systems with concentrated and distributed parameters. It has to be noted that the wave length ($\lambda_2 = 16.4751$ m) and the bioreactor length ($R = 5$ m) are of one and the same order. If D_X and D_S tend to zero, A_2 tends to zero too. In this case the considered nonlinear system is unstable regarding all kinds disturbances. The meaning of this fact is simple: at zero diffusion coefficients in the one-dimensional bioreactor with length (r) there is a copulation of identity cells, the symmetrical states of which are unstable [9]. When there is a diffusion the stability of the solutions describing the symmetrical states increases at small disturbances. This is naturally since the simultaneous exchange of the substratum and the product makes difficult the switching over of two neighbouring cells in different regimes. As a result the neighbouring cells are switched over in the regime of the second fixed point at the product diffusion. When the substratum concentration decreases the same cells are switched over in a converse direction at the substratum diffusion. In this way the regime of one or other cell is determined depending on the competition of two kind influences – specific (by product diffusion) and nonspecific (by substratum diffusion). If the concentration of the cells (X) becomes critical (effect of the "narrowness") it is possible to be reached to the first fixed point from a physical point of view, at the condition that the biotechnological process is not terminated. In conclusion this analysis shows that the space periodical and independent of time solutions (dissipative structure) in the distributed system can arise when there exists conditions guaranting the relaying invariant regarding time.

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Global Journal of Science Frontier Research
Physics & Space Science
Volume 12 Issue 3 Version 1.0 April 2012
Type : Double Blind Peer Reviewed International Research Journal
Publisher: Global Journals Inc. (USA)
Online ISSN: 2249-4626 & Print ISSN: 0975-5896

Reflection and Refraction of Bulk Exchange Spin Wave on the Interface of Two Ferromagnetic Media in Planar Magnetic Field

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GJSFR-A Classification: *FOR Code: 020404*

REFLECTION AND REFRACTION OF BULK EXCHANGE SPIN WAVE ON THE INTERFACE OF TWO FERROMAGNETIC MEDIA IN PLANAR MAGNETIC FIELD

Strictly as per the compliance and regulations of :

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S. Reshetnyak [α] & A. Berezhinsky [σ]

Abstract - Behavior of spin wave propagation in ferromagnetic medium with non-uniform distribution of magnetic parameters is studied. In particular, the influence of external magnetic field on behavior of bulk spin wave propagating through inhomogeneity made in form of lens (lens is biaxial ferromagnet placed into biaxial ferromagnetic medium with another magnetic parameters. Ferromagnets are in the homogeneous magnetic field directed along the hard axis) is studied.

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I. Introduction

Recent advances in nanotechnologies and nanoelectronics call for the creation of new devices utilizing the characteristic features of spin waves. Under these circumstances it is of interest to use the geometrical-optics approximation to describe the behavior of spin waves propagating in a medium with an ingomogeneous distribution of magnetic parameters. This paper is devoted to application of geometrical optics formalism [1] to the description of behavior of spin waves propagating in a ferromagnetic medium with non-uniform distribution of magnetic parameters. Use of this approach enables to obtain a necessary veering of propagation of spin waves (in particular, a focusing) with the help of artificial inhomogeneities of medium's magnetic parameters of the given configuration, and also by change of value of an external magnetic field.

II. Equations of Magnetization Dynamics

Let us consider an infinite ferromagnet consisting of two semi-infinite homogeneous parts that are in contact along the xOz plane. In the corresponding half-spaces, these parts of ferromagnet are characterized by the saturation magnetizations M_{01} and M_{02}, exchange interaction parameters α_1 and α_2, uniaxial magnetic anisotropy β_1 and β_2, as well as by rhombic magnetic anisotropy ρ_1 and ρ_2. The easy magnetization axis of each magnet is directed along the z axis.

The material is placed in an external uniform permanent magnetic field H_0, directed along the hard axis and the y axis of the coordinate system. Also plain $z = 0$ separates given structure from vacuum.

The energy density of such magnetic structure in exchange mode looks like

$$w = \sum_{j=1}^{2} \theta[(-1)^j y] w_j + A\delta(x)\mathbf{M}_1\mathbf{M}_2 \qquad (1)$$

where

$$w_j = \frac{\alpha_j}{2}\frac{\partial m_j}{\partial x_k}\frac{\partial m_j}{\partial x_k} - \frac{\beta_j}{2} m_{jz}^2 - \rho_2\left(m_{jx}^2 + m_{jz}^2\right) - H_0 M_{jy}, \qquad (2)$$

$\theta(x)$ is step function; $\mathbf{M}_j = M_{0j}\mathbf{m}_j$, $\mathbf{m}_j$ are unit vectors in the direction of magnetization, j=1,2; A is the constant describing a coupling on interface between half-spaces at y=0. Note that the case A=0 is equivalent to the absence of a coupling between layers through an interface, and $A \to \infty$ corresponds to an ideal (in a coupling sense) boundary [2].

Following [3] we represent the distribution of the magnetization in the material in the form

$$\mathbf{M}_j(\mathbf{r},t) = M_{0j}\,\psi_j^{+}(\mathbf{r},t)\,\boldsymbol{\sigma}\psi_j(\mathbf{r},t), \qquad (3)$$

where ψ_j denotes quasiclassical wave functions, which play the role of the order parameter of spin density, $\mathbf{r}$ is the radius vector in the Cartesian coordinate system, t is the time, and $\boldsymbol{\sigma}$ is a vector of Pauli matrices.
The Lagrange equations have the form

$$i\hbar\frac{\partial\psi_j(\mathbf{r},t)}{\partial t} = -\mu_0\mathbf{H}_{ej}(\mathbf{r},t)\,\boldsymbol{\sigma}\psi_j(\mathbf{r},t), \qquad (4)$$

where μ_0 is a Bohr magneton, $\hbar$ is the Plank constant,

and $\mathbf{H}_{ej} = -\frac{\partial w_j}{\partial \mathbf{M}_j} + \frac{\partial}{\partial x_k}\frac{\partial w_j}{\partial\left(\partial\mathbf{M}_j/\partial x_k\right)}$.

Then, using linear perturbation theory, the solution of Eq.(4) can be written as following

$$\Psi(\mathbf{r},t) = e^{i\eta t}\begin{pmatrix}1\\ i\end{pmatrix} + Ae^{i\eta t}\begin{pmatrix}\xi(\mathbf{r},t)\\ \chi(\mathbf{r},t)\end{pmatrix}, \qquad (5)$$

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where $\eta = \frac{\mu_0 H_0}{\hbar}$, and where $\xi(\mathbf{r},t)$, $\chi(\mathbf{r},t)$ are small additions characterizing the deviation of magnetization from the ground state.

Linearizing Eq.(4) and taking into account Eq.(2), we obtain

$$\xi = i\chi, \tag{6}$$

$$-\frac{\hbar^2}{\left(2\mu_0 M_{0j}\right)^2}\frac{\partial^2 \xi_j(\mathbf{r},t)}{\partial t^2} = \\ = \left[\alpha_j^2\Delta^2 + 2\alpha_j\left(\tilde{H}_{0j} - \beta_j/2 - \rho_j\right)\Delta + \right. \\ \left. + \left(\tilde{H}_{0j} - \rho_j\right)\left(-\tilde{H}_{0j} + \beta_j + \rho_j\right)\right]\xi_j(\mathbf{r},t), \tag{7}$$

where $\tilde{H}_{0j} = \frac{H_0}{M_{0j}}$.

Equation (7) describes the magnetization dynamics in the short-wavelength (exchange) approximation.

Using the approach [4] of geometrical optics, we obtain the refractive index of spin wave

$$n^{\pm} = \sqrt{\frac{\alpha_1}{\alpha_2}\frac{\beta_2/2 + \rho_2 - \tilde{H}_{02} \pm \sqrt{\Omega_2^2 + \beta_2^2/4}}{\beta_1/2 + \rho_1 - \tilde{H}_{01} \pm \sqrt{\Omega_1^2 + \beta_1^2/4}}}, \tag{8}$$

where $\Omega_j = \frac{\omega\hbar}{2\mu_0 M_{0j}}$.

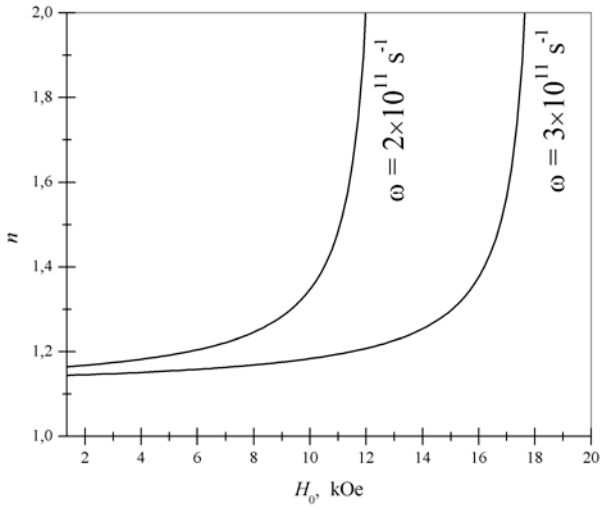

Fig.1 : Dependencies of refraction index of spin wave n on value of external homogeneous magnetic field H_0., $\alpha_1 = 7.4\times10^{-11}$ cm^2, $\alpha_2 = 5\times10^{-11}$ cm^2, $\beta_1 = 20$, $\beta_2 = 30$, $\rho_1 = 3$, $\rho_2 = 6$, $M_{01} = 90$ G, $M_{02} = 110$ G

Fig.1 shows dependency of refractive index on external magnetic field. As it can be seen from the figure it is possible to change refractive index of spin wave in a wide range of values by only changing of external magnetic field keeping constant the frequency and magnetic parameters of structure.

III. Reflection and Transmission Amplitudes

Let a spin wave to impinge on the interface from the homogeneous magnet with the parameter α_1 in the positive direction of y at an arbitrary angle.

Let's use boundary conditions for $\xi(\mathbf{r},t)$, which follow from (1)-(2):

$$\left[A\gamma\left(\xi_2 - \xi_1\right) + \alpha_1\xi_1'\right]_{y=0} = 0 \\ \left[A\left(\xi_1 - \xi_2\right) - \gamma\alpha_2\xi_2'\right]_{y=0} = 0. \tag{9}$$

Here $\gamma = M_{02}/M_{01}$. We shall obtain the expressions for amplitudes of spin wave reflection and transmission. Suppose, incident, reflected and transmitted waves are given by $\xi_I = \exp\left(i\left(\mathbf{k}_0\mathbf{r} - \omega t\right)\right)$, $\xi_R = R\exp\left(i\left(\mathbf{k}_1\mathbf{r} - \omega t\right)\right)$ and $\xi_D = D\exp\left(i\left(\mathbf{k}_2\mathbf{r} - \omega t\right)\right)$ correspondingly. Here R is a complex reflection amplitude, D is a transmission amplitude, $\mathbf{k}_0$, $\mathbf{k}_1$ are wave vectors of incident and reflected waves correspondingly, $\mathbf{k}_2$ is a wave vector of transmitted wave. Then

$$R = \frac{k_0\alpha_1\cos\theta_1 B - iA\left(\alpha_1\cos\theta_1 - \gamma B\right)}{k_0\alpha_1\cos\theta_1 B - iA\left(\alpha_1\cos\theta_1 + \gamma B\right)}, \\ D = \frac{-2iA\alpha_1\cos\theta_1}{k_0\alpha_1\cos\theta_1 B - iA\left(\alpha_1\cos\theta_1 + \gamma B\right)}, \tag{10}$$

where $B = \alpha_2\gamma\sqrt{n^2 - \sin^2\theta_1}$. The "±" sign next to n is neglected for simplicity.

In the case of an ideal boundary ($A \to \infty$) Eqs. (10) can be rewritten as

$$R = \frac{\alpha_1\cos\theta_1 - \alpha_2\gamma^2\sqrt{n^2 - \sin^2\theta_1}}{\alpha_1\cos\theta_1 + \alpha_2\gamma^2\sqrt{n^2 - \sin^2\theta_1}}, \\ D = \frac{2\alpha_1\cos\theta_1}{\alpha_1\cos\theta_1 + \alpha_2\gamma^2\sqrt{n^2 - \sin^2\theta_1}}, \tag{11}$$

IV. Estimations for The Parameters of Spin-Wave Lenses

Let's give the estimations for material's parameters when a lens is thin. Obviously, we have to provide a necessary lens transparency.

Let's consider that exchange parameters A_1 and A_2 ($A_j = \alpha_j M^2/2$ [3]) are equal for both half-spaces. In this case $\alpha_1 = \alpha_2\gamma^2$ and Eqs. (11) can be reduced to

$$R = \frac{\cos\theta_1 - \sqrt{n^2 - \sin^2\theta_1}}{\cos\theta_1 + \sqrt{n^2 - \sin^2\theta_1}}, \qquad D = \frac{2\cos\theta_1}{\cos\theta_1 + \sqrt{n^2 - \sin^2\theta_1}}. \tag{12}$$

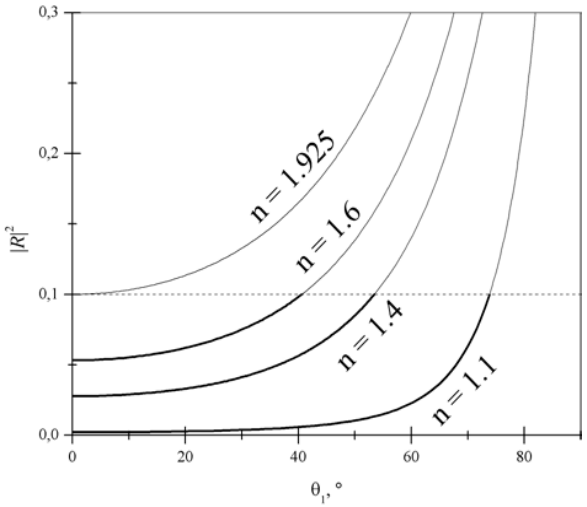

Fig.2A : Dependencies of intensity of reflected wave $|R|^2$ on the incident angle θ_1 for $1<n<2$

In Fig.2A and Fig.2B we show the dependencies of intensity of reflected wave $|R|^2$ on the incident angle θ_1 for different values of refractive index n. It can be seen that intensity depends strongly on the incident angle and intensity has the lowest values at small angles.

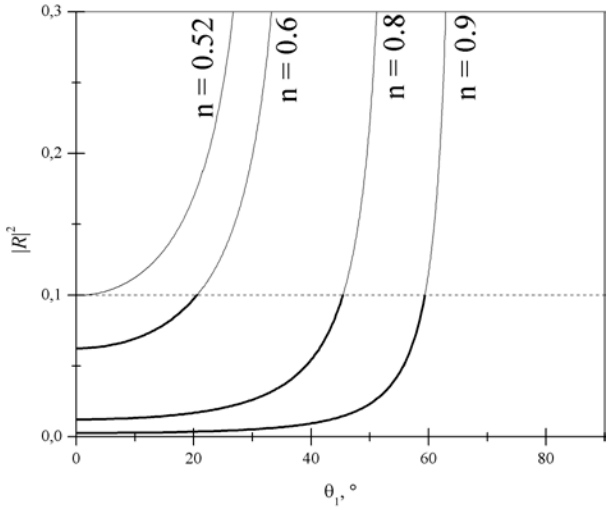

Fig.2B : Dependencies of intensity of reflected wave $|R|^2$ on the incident angle θ_1 for $0.5<n<1$

In case of small incident angles Eq. (11) can be rewritten as

$$R = \frac{\alpha_1 - \alpha_2\gamma^2 n}{\alpha_1 + \alpha_2\gamma^2 n}, \qquad D = \frac{2\alpha_1}{\alpha_1 + \alpha_2\gamma^2 n}. \tag{13}$$

Demanding a conformity to the condition $|R|^2 < \eta$, where η is a necessary smallness of reflection coefficient, to provide enough transparency of lens, we obtain a limitation on n and, therefore, on α, β, ρ, ω, M_0 and H_0:

$$\frac{1-\sqrt{\eta}}{1+\sqrt{\eta}} < \frac{\alpha_2\gamma^2}{\alpha_1} n < \frac{1+\sqrt{\eta}}{1-\sqrt{\eta}} \tag{14}$$

In particular, in case of $\alpha_1 = \alpha_2\gamma^2$ reflection coefficient is less then 10% if $0.52<n<1.92$.

By adjusting the relation $\alpha_2\gamma^2/\alpha_1$ one can set up the lens for working with particular refraction index. Indeed, using Eq. (13) we obtain

$$\frac{\alpha_2\gamma^2}{\alpha_1} \to \frac{1}{n}, \text{ when } \theta_1 \to 0 \text{ and } |R|^2 \to 0. \tag{15}$$

For example, if one is going to use values of refractive index that are close to $n \approx 2$, then he should choose relation $\alpha_2\gamma^2/\alpha_1$ to be close to 0.5. In this case reflection coefficient is less then 10% if $1.04<n<3.85$ (Fig. 3).

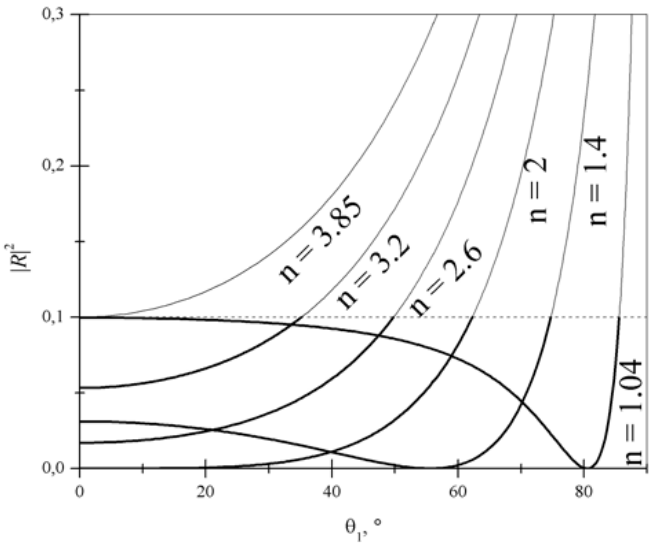

Fig.3 : Dependencies of intensity of reflected wave $|R|^2$ on the incident angle θ_1 for $1.04<n<3.85$

V. Conclusion

We have shown that it is possible to change "optical" parameters of spin-wave lens in a wide range of values by only changing of the external magnetic field keeping constant the frequency and magnetic parameters of structure. This fact allows one to use the results of this research in applications of spin-wave electronics.

It is also shown that despite the strong dependence of reflection coefficient on incident angle it is possible to obtain suitable reflection coefficient by adjusting magnetic parameters of the structure.

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Global Journal of Science Frontier Research
Physics & Space Science
Volume 12 Issue 3 Version 1.0 April 2012
Type : Double Blind Peer Reviewed International Research Journal
Publisher: Global Journals Inc. (USA)
Online ISSN: 2249-4626 & Print ISSN: 0975-5896

Magnetic Characteristics Measurements In Htc Super - conductors

By J. Sosnowski & H. Malinowski
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Abstract - Selected methods for measurements magnetic quantities in HTc superconductors are discussed. First one is based on an analysis of the magnetic hysteresis curves, while second follows from the investigations of the dynamic anomalies of the current-voltage characteristics in slowly varying magnetic field.

GJSFR-A Classification: *FOR Code: 020404*

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Magnetic Characteristics Measurements In Htc Superconductors

J. Sosnowski [α] & H. Malinowski [σ]

Abstract - Selected methods for measurements magnetic quantities in HTc superconductors are discussed. First one is based on an analysis of the magnetic hysteresis curves, while second follows from the investigations of the dynamic anomalies of the current-voltage characteristics in slowly varying magnetic field.

I. Introduction

High temperature oxide superconductors are characterised by peculiar magnetic properties, allowing treat them as unique magnetic materials. They are diamagnetic materials for small applied increasing magnetic field but indicate too, from other side giant trapped magnetic flux in reverse direction. It allows consider these superconductors as very efficient permanent magnets.

Magnetic characteristics of superconductors are related to very peculiar form of the penetration of magnetic flux into these materials in the form of vortices - flux lines or pancake shape, each of them transports lowest known value of quantized magnetic flux $\Phi_0 = 2{,}067 \cdot 10^{-15}$ Wb. Such small quantity of magnetic flux allows use superconducting materials for construction of ultra sensitive devices for detecting lowest magnetic fields. In the paper two methods of detecting magnetic quantities in HTc superconductors are discussed: first one follows from the magnetization hysteresis curves measurements and second for which only first results were received until now, is based on the dynamic anomalies of the current-voltage characteristics measurements.

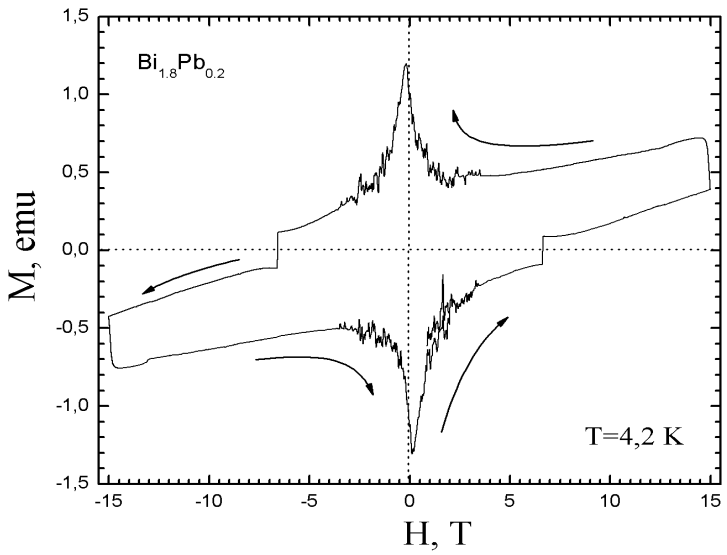

Fig. 1 : Full hysteresis loop of the magnetization curve in high magnetic field, of sintered HTc superconductor $Bi_{1.8}Pb_{0.2}Sr_2Ca_2Cu_3O_{10}$ composition as a function of applied magnetic induction. Arrows indicate the direction of variation of applied magnetic field. Measurement performed by dr. D. Gajda from MLSPMiNT.

II. Experimental Results

Example of the magnetic hysteresis curve measured on sintered HTc superconductor of the $Bi_{1.8}Pb_{0.2}Sr_2Ca_2Cu_3O_{10}$ composition is shown in Fig. 1. Large irreversibility of hysteresis loop is observed here as well as numerous instabilities of magnetic induction distribution, which in uncontrolled way can lead to rapid transition of superconductor into the normal state. Partial flux jumps in superconductors are therefore in some sense analogous phenomenon to Barkhausen noises appearing in magnetic materials. Magnetization measurements allow to determine most of the magnetic quantities of HTc superconducting materials, including magnetic critical fields but also critical currents, magnitude of trapped magnetic induction, magnetic hysteresis losses and other parameters. Experimentally magnetization curves are measured frequently by using vibrating sample magnetometer, which method is now

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the subject of the standardization procedure, according to the standard IEC EN 61788-13. In this method sample is vibrating in longitudinal magnetic field generated by superconducting electromagnet. Induced in the pick-up coils signal, directly proportional to the magnetic moment of the superconductor is given onto the power amplifier and registered in the computer unit in the function of an applied magnetic field. Area of the magnetization curve hysteresis loop, shown in Fig. 1 determines the losses generated in bulk superconductor during closed cycle of magnetic field. Irreversibility of the magnetization curve observed in measurements, determines the critical current density of the superconductor j_c, according to the relation joining the hysteretic magnetization of the superconducting pellet of the diameter D, with its critical current density: $M = j_c \cdot D$, received in the Bean's critical state model [1]. Magnetization M is important magnetic quantity allowing to determine also the levitation force F between two magnetic materials characterized by the magnetization values M_1 and M_2 respectively, which is essential parameter of the superconducting bearings: $F = M_1 M_2 / (2\mu_0)$, where μ_0 is magnetic permeability. According to above considerations it is clear too that most attractive for using in the superconducting bearings and levitating devices are superconducting macromolecules, which can reach the dimension even up to 10 cm.

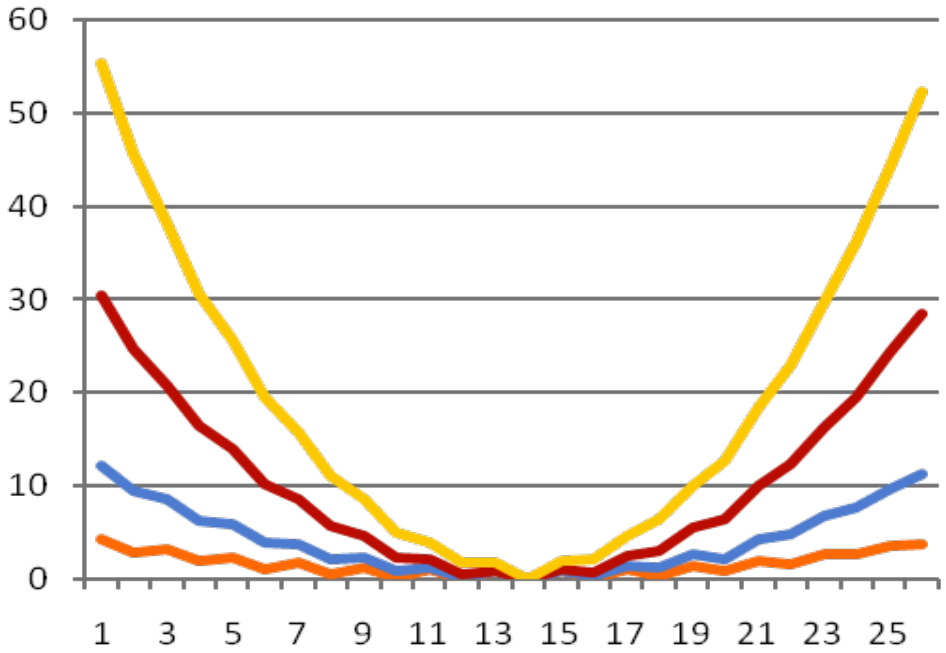

Fig. 2 : Profiles of the measured deflection along an axis of superconducting coil with inserted inside HTc shield, of magnetic induction distribution from the maximal value, in relative units. Subsequent curves from bottom are given for increasing magnetic induction: 0.1T, 0.2T, 0.5T, 1T

Diamagnetic features of superconductors, observed especially in low magnetic field, are useful for construction of the magnetic shields, allowing to homogenize the magnetic induction distribution of the superconducting electro-magnets. An example of measurements the profiles of magnetic induction inside the superconducting coil with inserted inside superconducting HTc shield is shown in Fig. 2. Observed here small steps in magnetic induction profile, especially well seen at low applied magnetic field, reflect the structure and shielding properties of this superconducting thin coil, formed from wound spirally single layer of HTc superconducting tape of the first generation. The length of this tape L, of the width b and thickness a, necessary for construction of HTc superconducting shield of the inner radius R, thickness $T = \frac{\Delta B a b}{\mu_0 I_C}$ and length C screening magnetic induction ΔB, is connected with critical current IC of this tape according to the relation:

$$L = \frac{2\pi C b \Delta B}{\mu_0 I_C}\left(R + \frac{a}{2}\left(\frac{b\Delta B}{\mu_0 I_C} - 1\right)\right) \qquad (1)$$

III. Modeling of Dynamic Current-Voltage Characteristics of HTC Superconductors in Varying Magnetic Field

Measurements of magnetization curves allow in inductive way determine essential electro-magnetic quantities characterizing HTc superconductors, including critical current. This essential parameter of superconductors is determined directly in resistive way from current-voltage curves, assuming appropriate

voltage or resistivity criterion. In this clause we consider the I-V characteristics in slowly varying magnetic induction. Then dynamic current-voltage characteristics anomalies we have observed previously: normal and inverse one [2], as is shown in Fig. 3. These anomalies should be useful as a new tool for detecting magnetic quantities in superconductors – especially describing the magnetic flux penetration and concerning therefore the stability behavior of magnetic induction in HTc superconductors.

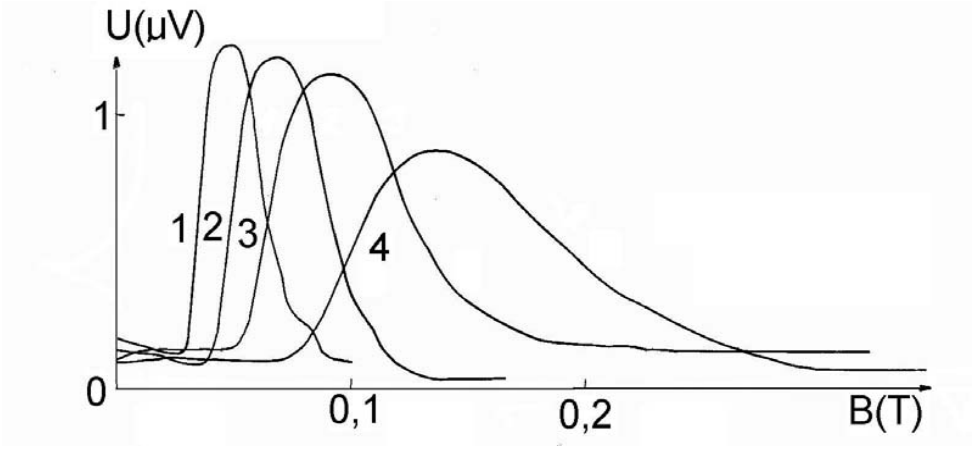

Fig. 3 : Measured dynamical anomalies of I-V curves on YBaCuO bulk superconductor for various values of the linearly time-varying magnetic field: (1) 1 mT/s, (2) 5 mT/s, (3) 10 mT/s, (4) 15 mT/s

Theoretical analysis of this phenomenon has been performed in two ways, basing on generalized critical state model received, while taking into account in details the nano-sized pinning centre-vortex interaction [1] and by considering the diffusion equation. In the critical state model the critical current magnetic field dependence has been then assumed as:

$$\mu_0 j_c = \pm \frac{\alpha}{\left(B(x) + B^0\right)^{\gamma}} \qquad (2)$$

where $\mu_0$is magnetic permeability α and B^o material parameters, while γ varies between 0 and 1. Generated electric field has been calculated separately for non-saturated case, it is when magnetic induction does not penetrate into the centre of the superconducting slab, while both branches of the magnetic induction do not meet together and saturated case of total flux penetration. For non-saturated case in generalized pinning force model and saturated one, induced electric fields are described by relations 3 and 4 respectively:

$$E = \frac{\dot{B}}{\alpha}\left(B + \Delta B + B^0\right)^{\gamma} \cdot \left\langle \left[\left(B + \Delta B + B^0\right)^{1+\gamma} - \alpha(1+\gamma)x_m\right]^{\frac{1}{1+\gamma}} - B^0 \right\rangle \qquad (3)$$

$$E = \frac{\dot{B}}{\alpha}\left\langle \left(B + \Delta B + B^0\right)^{\gamma} \cdot \left(\left[\left(B + \Delta B + B^0\right)^{1+\gamma} - \alpha(1+\gamma)x_m\right]^{\frac{1}{1+\gamma}} - B_{av}(x_m) \right) + B^1\left(B_{av}(x_m) - B^0\right) \right\rangle \qquad (4)$$

In Eqs. 3-4 symbol B denotes time dependent applied magnetic induction, while $\dot{B} = \partial B / \partial t$ its time derivative, while x_m sample half-thickness. ΔB is magnetic induction shift on the surface of superconductor connected with the transport current flow, while functions B_{av} and B^1 are related to the shift of magnetic induction in the middle of the superconductor and on its surface in dependence on the amplitude of the transport current.

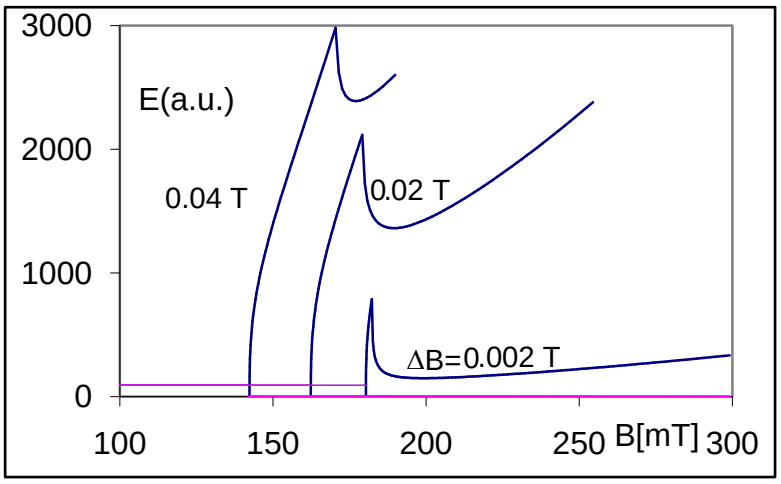

Fig. 4 : Calculated influence of transport current expressed here by ΔB on dynamic I-V curves anomalies in slowly varying magnetic field.

Results of calculations according to relations 3-4, dynamical current-voltage characteristics anomalies in this model, in the function of transport current amplitude flowing through the HTc superconductor, expressed by parameter ΔB, are shown in Fig. 4. Above anomalies as shows Fig. 3 are also sensitive to magnetic field sweep rate, as well as magnetic field dependence of critical current. Similar results are received after solving the magnetic diffusion equation, mentioned previously, which indicates on general form of observed phenomenon, which can be useful therefore as new tool for detecting such dynamic magnetic quantities as magnetic field sweep rate, current amplitude and its frequency, flux diffusion velocity, sample quality.

Acknowledgment

Authors are grateful to dr. V.I. Datskov and dr D. Gajda for experimental collaboration.

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Global Journal of Science Frontier Research
Physics & Space Science
Volume 12 Issue 3 Version 1.0 April 2012
Type : Double Blind Peer Reviewed International Research Journal
Publisher: Global Journals Inc. (USA)
Online ISSN: 2249-4626 & Print ISSN: 0975-5896

Fluorescence, In Microscopy and Imaging

By P. N. Dikedi
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Abstract - This is a swift report on fluorescence and its application as a tool in imaging and microscopy; to properly comprehend this subject, with the aid of the Jablonski diagram, brief descriptions and discussions are given on fluorescence; rhodamine 6G homo-FRET reaction is considered from which both the absorption and emission spectra are drawn on a graph. Additionally, the wealth of applications of fluorescence imaging techniques such as Fluorescence Lifetime Imaging Microscopy (FLIM) and Fluorescence Polarisation and Anisotropy techniques are considered. Applications of molecular imaging techniques in cell biology and medical science are mentioned.

GJSFR-A Classification: FOR Code: 020402

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Fluorescence, In Microscopy and Imaging

P. N. Dikedi

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I. Introduction

The aim of this report is to discuss the principle of fluorescence, and to unravel its inevitable use as a tool in imaging and microscopy. A useful feature of fluorescence is high sensitivity detection; which is its key advantage as an imaging tool. It is well reported that the fluorescence spectra from photo sensitizers can act as image guiding tool in differentiating malignant tissues from normal ones; additionally fluorescent signatures could be used to differentiate between malignant and benign diseases [1]. In section 2, the phenomenon of fluorescence will be discussed, in section 3, a brief explanation of the Jablonski diagram, will be given; thereafter in section 4, we shall probe into fluorescence imaging and microscopy, discussing its valuable applications in cell biology and medical science. Conclusions will be drawn in section 5.

II. Fluorescence

In initiating brief discussions on fluorescence, it does a lot good to start by defining what Luminescence is; it is the emission of light from any substance and it occurs from an electronically excited state. Luminescence is divided into two parts: fluorescence and phosphorescence.

One can now proceed to briefly discuss Fluorescence as a type of luminescence—which is short lived—created by electromagnetic excitation, involving absorption of light by a fluorophore—a fluorescing functional group—at a higher energy or shorter wavelength, followed by emission of light at a lower energy or longer wavelength. This process occurs at a rate called the rate of fluorescence, which is about $10^{8}s^{-1}$. Since fluorescence process involves occurrences of emission and absorption, it is important to note that time elapses between both occurrences, hence the length of time between emission and absorption or the average time between when a fluorophore is excited and when it returns to the ground state is referred to as fluorescence lifetime; this time lies between 10^{-9} and 10^{-8}s and it is a relatively short time indeed—a further discussion on this will be given in section 4.

When emission persists longer after excitation light has been extinguished, then, this phenomenon is referred to as phosphorescence—this process is not the focus for discussion in this paper and so will be left-off. Fluorescence as a tool in imaging and microscopy is well reported by Klaus *et al* (2004)[2]; fluorescence imaging techniques are optical imaging techniques which find their applications in biomedical and biological sciences because they are applicable to live cells and tissue probing in such a manner that the fluorophore environment need not be compromised with biochemical assays.

Fluorophores are molecules or functional groups which are capable of fluorescing; they are used—or selected for use—in terms of their quantum yields. Quantum yield of a fluorophore is the ratio of the number of emitted photons to the number of absorbed photons; this is expressed as:

$$\emptyset = \frac{\tau}{\tau_0} = \frac{k_r}{k_r + k_{nr}}$$

where, τ_0, is the natural or radiative lifetime, k_r and k_{nr}, are the radiative and nonradiative decay rate constants, respectively.

The highest possible quantum yield is unity or 100%, and fluorophores with high quantum yields are well sought after because of their great relevance in the biological sciences and chemistry. Fluorescein and Rhodamine 101 can each attain a quantum yield of 0.92 and 1 respectively. In discussing further on fluorescence, it is important to delve briefly into Fluorescence resonance/Förster energy transfer (FRET) phenomenon; this phenomenon is a radiationless energy transfer between two molecules, as close as < 10 nm. This is illustrated by a fluorescent emission spectra; the occurrence of FRET is illustrated by the overlaps of the emission spectrum of the donor molecule and that of the acceptor molecule.

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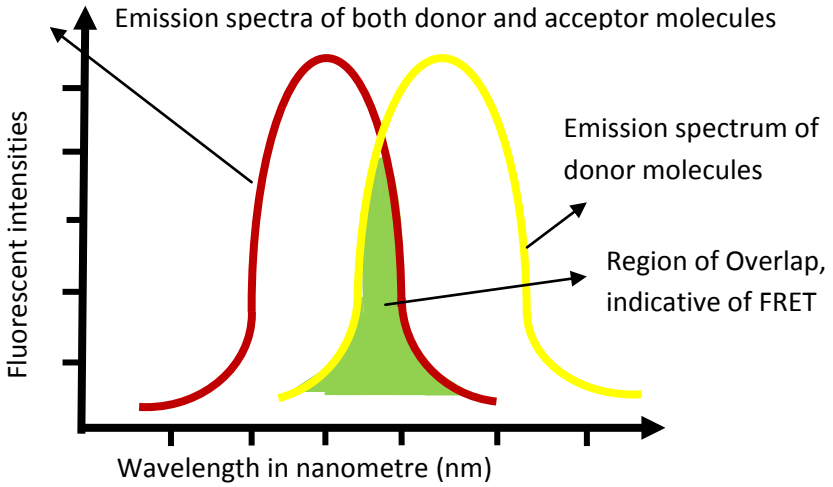

Figure 1 : A schematic of the fluorescent emission spectra with overlaps of the donor and acceptor spectra indicating FRET.

Figure 1 is a schematic of an arbitrary emission and absorption spectra; the green shaded region, an overlap of the spectra, represents spectral overlap integral.

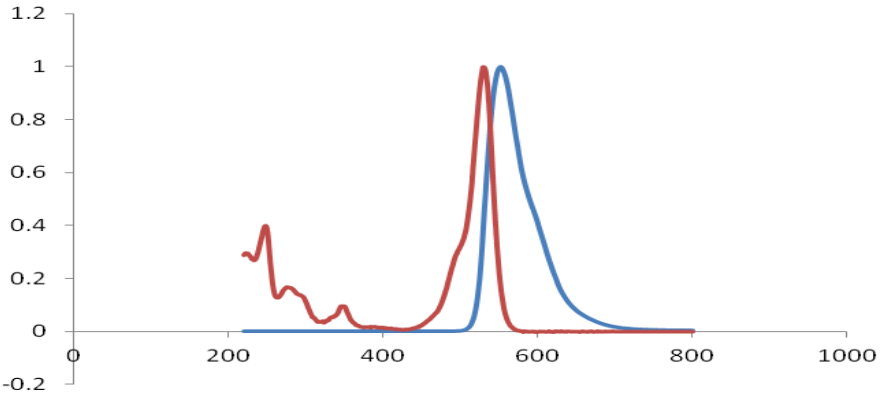

Fig. 2 : Normalized emission-absorption spectra for Rhodamine 6G Homo-FRET reaction

Fluorescent emission spectra are a plot of fluorescence intensities versus wavelength or wave numbers. They are a function of the chemical structure of a fluorophore.

Examples of these spectra are those of Rhodamine 6G homo-FRET.

Figure 2 is a schematic of the absorption and emission spectra for homo-FRET reaction of Rhodamine 6G; wavelength values ranges between $4.90x10^4$nm and $8.00x10^4$nm and corresponding molar extinction values include from $1.314874x10^4$ to $7.392346x10^4$. Below is a very simplified tabulation pertinent to the schematics in figure 2. Below is a selection from the groups of wavelengths, intensities and normalised intensities.

Table 1: shows selected values of wavelengths, intensities and normalised intensities of Rhodamine 6G for both absorption and emission spectra

ABSORPTION			EMISSION		
Wavelengths (nm)	Intensities	Normalised intensities	Wavelengths (nm)	Intensities	Normalised intensities
600	0.00006	4.07039E-05	600	8.38 X10^7	0.406225
595	0.00023	0.000156032	595	9.29 X10^6	0.450169
590	0.00047	0.000318847	590	1.01 X10^7	0.491429

585	-0.00018	-0.00012211	585	1.11 X10^7	0.538
580	0.00201	0.001363581	580	1.23 X10^7	0.594328

III. Jablonski Diagram and Photophysical Processes

The Jablonski diagram, a schematic, describes a series of photo physical occurrences, due to absorption of energy by a photon; these occurrences include: fluorescence, phosphorescence, intersystem crossing—which occurs from a singlet to triplet state—and internal conversion or vibration relaxation, in which energy is lost without emission of light [3].

A few parameters which help in describing the above mentioned processes are worth the mention; one of such is the decay rate constant, k, which describes the probability of each process taking place.

Another is the mean lifetime, τ, which is the time required for a molecule or a set of molecules to decay from one state to another. Both parameters are inversely related to each other and are described by:

$$k = \frac{1}{\tau}$$

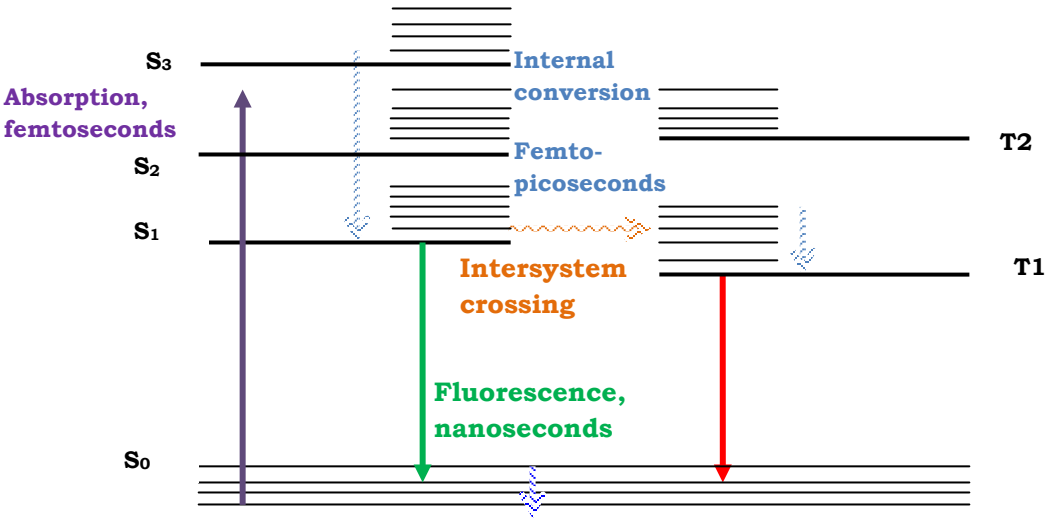

Figure 1 : An adopted Schematic of the Jablonski diagram elaborating photophysical processes [3]

It is also the time for N excited molecules to reduce by a factor, e, so that lifetime for fluorescence and other nonradiative processes also called fluorescence lifetime could be described as the time for a population of excited fluorophores to reduce exponentially to N/e.The lifetimes for fluorescence, phosphorescence and internal conversion processes are in nanoseconds (ns), microseconds (μs) and tens of femtoseconds (fs), respectively.

The expression for lifetime, in section 3, could also be expressed in an extended form—so to speak—as:

$$\tau = \frac{1}{k_r + k_{nr}},$$

Fluorescence decay time depends both on the intrinsic characteristics of the fluorophore and its local environment; local viscosity, PH, or refractive index and molecular interaction all of which affect the fluorescence decay time.

IV. Applications of Fluorescence Imaging and Microscopy

A number of fluorescence imaging techniques and their applications apposite to medical and biological sciences are either in use or underway. A few of the many applications of these techniques are presented in the following subsections:

a) Molecular imaging

This technique is employed in molecular imaging; this imaging aims to detect, localise and monitor molecular processes by the use of sensitive instruments.

Though they find their major use in clinical chemistry and *in vitro* biological analysis by measuring biological response; this technique is useful in assessing the internal environment of fluorescent probes; additionally, molecular interactions can be determined via its application as a biological imaging tool.

Fluorescence molecular probes are being designed to monitor intracellular PH—they employ ratiometric measuring method; tissues which surround tumours and diseased cells generally show abnormal pH from the rest tissues and cells and hence are detected [4]. In cell biology, abnormal PH values could impair the proper functioning of subunits of a cell such as plant vacuoles and endosomes and in medical science, they could lead to abnormal cell growth and division, a situation akin to those observed in disease types such as cancer and Alzheimer; variations in the PH value could also affect the nervous system by distrupting the synaptic transmission. The need for a qualitative measurement of PH arises; this measurement is provided by fluorescent indicators which switch off and on.

Some of the fluorescent sensors used for intra cellular PH measurements include but are not limited to, 2′,7′-Bis-(2-carboxyethyl)-5-(and-6-)-carboxyfluorescein **4** (BCECF),2′,7′-bis-(2-carboxypropyl)-5-(and-6-)-carboxy-fluorescein (BCPCF) , Fluorescein and Fluorescein sulfonic acid [5]

b) Fluorescence polarization and anisotropy

Light made to pass through polarisers, which eventually illuminate fluorophores, produces polarised fluorescence—a type of polarised emission. Polarisation, P, is related to the observed parallel and perpendicular intensities, $I\perp$ and $I\parallel$ respectively by:

$$P = \frac{I\parallel - I\perp}{I\parallel + I\perp}$$

Anisotropy, denoted by r, is another terminology under polarised emission and it is related to $I\perp$ and $I\parallel$ by:

$$r = \frac{I\parallel - I\perp}{I\parallel + 2I\perp}$$

Polarisation and anisotropy are related to each other by the following expression:

$$r = \frac{2}{3}\left(\frac{1}{P} - \frac{1}{3}\right)^{-1}$$

Fluorescence polarisation and anisotropy technique has its great relevance in clinical and biomedical fields. In the pharmaceutical industry, the discovery process of a compound of great therapeutic benefit can be a time consuming and an arduous task. Since the amount of potential molecules which could provide such benefits are overwhelming—up to millions of compounds, hence the need for a swift high-throughput screening technique arises. Fluorescence polarisation and anisotropy technique is being considered as such high-throughput screening technique which has the potential to deliver in terms of both accuracy and speed [6]

This method is strongly reputable in the study of ligand binding—binding of small molecules to proteins. Binding of molecules like acridine, naphthalene dyes, xanthenes to bovine serum albumin (BSA) have been studied.

c) Fluorescence Lifetime Imaging Microscopy (FLIM)

Fluorescence Lifetime Imaging Microscopy (FLIM), a time resolved technique for acquiring images are of two categories; the first, is the confocal scanning or multiphoton excitation technique and the second is the wide-field camera based FLIM. This technique have been employed as a tool for identifying Förster Resonance Energy Transfer (FRET), at the instance of interactions between DNA, RNA, lipids, proteins and enzymes. As cited by Klaus *et al*, steady state anisotropy-a time resolved fluorescence anisotropy technique—has been used for contrasting between Fluorescein and GFP in a cell owing to their dissimilar anisotropies in terms of their molecular sizes. Homo-FRET can be detected by employing this technique. This technique is applicable to cell imaging; it shows image contrast by utilising spatial variations in fluorescence lifetimes in single cells. Unlike time resolved measurements which are sensitive to molecular movements and interactions, molecular information can be visualised in single cells. By employing this technique, the extent of fusion of endosomes in individual cells, have been observed [7].

FLIM system has been designed and built [8]; it is specifically for intraoperative disease diagnosis. By employing a flexible imaging probe—made up of a fibre bundle and gradient index objective lens—and an intensified CCD, tissue auto fluorescence—at 33ns excitation—was imaged. Contrast in fluorescence lifetime was shown between tumour (1.77+/-0.26ns) and normal (2.50+/-0.36ns) tissue. This confirms the potential usefulness of (FLIM) technique for diagnosing intra operative diseases.

V. Conclusions

Fluorescence processes have been mentioned. Applications of FLIM and fluorescent polarisation and anisotropy have been considered as imaging and microscopic tools; additionally, molecular imagings in which fluorescent PH sensors are used for intra cellular PH measurements, in the field of cell biology and medical science have been discussed. The future of fluorescence imaging technique is far from being bleak; its applications are on the rise.

VI. Acknowledgements

My first acknowledgement goes to God, *The fountain of Living Water* without whom I would have amounted to nothing, for seeing and keeping me through in the journey of life.

I am forever grateful for the rare unleashes of my mother and friend, Mrs. Luciana Dikedi, who passed on at 74, owing to a peripheral vascular disease and ascending feet gangrene.

My acknowledgement also extends to Dr. Klaus Suhling for rendering support by supplying some academic materials relating to this very short report.

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Final Points:

A purpose of organizing a research paper is to let people to interpret your effort selectively. The journal requires the following sections, submitted in the order listed, each section to start on a new page.

The introduction will be compiled from reference matter and will reflect the design processes or outline of basis that direct you to make study. As you will carry out the process of study, the method and process section will be constructed as like that. The result segment will show related statistics in nearly sequential order and will direct the reviewers next to the similar intellectual paths throughout the data that you took to carry out your study. The discussion section will provide understanding of the data and projections as to the implication of the results. The use of good quality references all through the paper will give the effort trustworthiness by representing an alertness of prior workings.

Writing a research paper is not an easy job no matter how trouble-free the actual research or concept. Practice, excellent preparation, and controlled record keeping are the only means to make straightforward the progression.

General style:

Specific editorial column necessities for compliance of a manuscript will always take over from directions in these general guidelines.

To make a paper clear

· Adhere to recommended page limits

Mistakes to evade

- Insertion a title at the foot of a page with the subsequent text on the next page

- Separating a table/chart or figure - impound each figure/table to a single page
- Submitting a manuscript with pages out of sequence

In every sections of your document

· Use standard writing style including articles ("a", "the," etc.)

· Keep on paying attention on the research topic of the paper

· Use paragraphs to split each significant point (excluding for the abstract)

· Align the primary line of each section

· Present your points in sound order

· Use present tense to report well accepted

· Use past tense to describe specific results

· Shun familiar wording, don't address the reviewer directly, and don't use slang, slang language, or superlatives

· Shun use of extra pictures - include only those figures essential to presenting results

Title Page:

Choose a revealing title. It should be short. It should not have non-standard acronyms or abbreviations. It should not exceed two printed lines. It should include the name(s) and address (es) of all authors.

Abstract:

The summary should be two hundred words or less. It should briefly and clearly explain the key findings reported in the manuscript--must have precise statistics. It should not have abnormal acronyms or abbreviations. It should be logical in itself. Shun citing references at this point.

An abstract is a brief distinct paragraph summary of finished work or work in development. In a minute or less a reviewer can be taught the foundation behind the study, common approach to the problem, relevant results, and significant conclusions or new questions.

Write your summary when your paper is completed because how can you write the summary of anything which is not yet written? Wealth of terminology is very essential in abstract. Yet, use comprehensive sentences and do not let go readability for briefness. You can maintain it succinct by phrasing sentences so that they provide more than lone rationale. The author can at this moment go straight to

shortening the outcome. Sum up the study, with the subsequent elements in any summary. Try to maintain the initial two items to no more than one ruling each.

- Reason of the study - theory, overall issue, purpose
- Fundamental goal
- To the point depiction of the research
- Consequences, including definite statistics - if the consequences are quantitative in nature, account quantitative data; results of any numerical analysis should be reported
- Significant conclusions or questions that track from the research(es)

Approach:

- Single section, and succinct
- As a outline of job done, it is always written in past tense
- A conceptual should situate on its own, and not submit to any other part of the paper such as a form or table
- Center on shortening results - bound background information to a verdict or two, if completely necessary
- What you account in an conceptual must be regular with what you reported in the manuscript
- Exact spelling, clearness of sentences and phrases, and appropriate reporting of quantities (proper units, important statistics) are just as significant in an abstract as they are anywhere else

Introduction:

The **Introduction** should "introduce" the manuscript. The reviewer should be presented with sufficient background information to be capable to comprehend and calculate the purpose of your study without having to submit to other works. The basis for the study should be offered. Give most important references but shun difficult to make a comprehensive appraisal of the topic. In the introduction, describe the problem visibly. If the problem is not acknowledged in a logical, reasonable way, the reviewer will have no attention in your result. Speak in common terms about techniques used to explain the problem, if needed, but do not present any particulars about the protocols here. Following approach can create a valuable beginning:

- Explain the value (significance) of the study
- Shield the model - why did you employ this particular system or method? What is its compensation? You strength remark on its appropriateness from a abstract point of vision as well as point out sensible reasons for using it.
- Present a justification. Status your particular theory (es) or aim(s), and describe the logic that led you to choose them.
- Very for a short time explain the tentative propose and how it skilled the declared objectives.

Approach:

- Use past tense except for when referring to recognized facts. After all, the manuscript will be submitted after the entire job is done.
- Sort out your thoughts; manufacture one key point with every section. If you make the four points listed above, you will need a least of four paragraphs.
- Present surroundings information only as desirable in order hold up a situation. The reviewer does not desire to read the whole thing you know about a topic.
- Shape the theory/purpose specifically - do not take a broad view.
- As always, give awareness to spelling, simplicity and correctness of sentences and phrases.

Procedures (Methods and Materials):

This part is supposed to be the easiest to carve if you have good skills. A sound written Procedures segment allows a capable scientist to replacement your results. Present precise information about your supplies. The suppliers and clarity of reagents can be helpful bits of information. Present methods in sequential order but linked methodologies can be grouped as a segment. Be concise when relating the protocols. Attempt for the least amount of information that would permit another capable scientist to spare your outcome but be cautious that vital information is integrated. The use of subheadings is suggested and ought to be synchronized with the results section. When a technique is used that has been well described in another object, mention the specific item describing a way but draw the basic

principle while stating the situation. The purpose is to text all particular resources and broad procedures, so that another person may use some or all of the methods in one more study or referee the scientific value of your work. It is not to be a step by step report of the whole thing you did, nor is a methods section a set of orders.

Materials:

- Explain materials individually only if the study is so complex that it saves liberty this way.
- Embrace particular materials, and any tools or provisions that are not frequently found in laboratories.
- Do not take in frequently found.
- If use of a definite type of tools.
- Materials may be reported in a part section or else they may be recognized along with your measures.

Methods:

- Report the method (not particulars of each process that engaged the same methodology)
- Describe the method entirely
- To be succinct, present methods under headings dedicated to specific dealings or groups of measures
- Simplify - details how procedures were completed not how they were exclusively performed on a particular day.
- If well known procedures were used, account the procedure by name, possibly with reference, and that's all.

Approach:

- It is embarrassed or not possible to use vigorous voice when documenting methods with no using first person, which would focus the reviewer's interest on the researcher rather than the job. As a result when script up the methods most authors use third person passive voice.
- Use standard style in this and in every other part of the paper - avoid familiar lists, and use full sentences.

What to keep away from

- Resources and methods are not a set of information.
- Skip all descriptive information and surroundings - save it for the argument.
- Leave out information that is immaterial to a third party.

Results:

The principle of a results segment is to present and demonstrate your conclusion. Create this part a entirely objective details of the outcome, and save all understanding for the discussion.

The page length of this segment is set by the sum and types of data to be reported. Carry on to be to the point, by means of statistics and tables, if suitable, to present consequences most efficiently.You must obviously differentiate material that would usually be incorporated in a study editorial from any unprocessed data or additional appendix matter that would not be available. In fact, such matter should not be submitted at all except requested by the instructor.

Content

- Sum up your conclusion in text and demonstrate them, if suitable, with figures and tables.
- In manuscript, explain each of your consequences, point the reader to remarks that are most appropriate.
- Present a background, such as by describing the question that was addressed by creation an exacting study.
- Explain results of control experiments and comprise remarks that are not accessible in a prescribed figure or table, if appropriate.
- Examine your data, then prepare the analyzed (transformed) data in the form of a figure (graph), table, or in manuscript form.

What to stay away from

- Do not discuss or infer your outcome, report surroundings information, or try to explain anything.
- Not at all, take in raw data or intermediate calculations in a research manuscript.

- Do not present the similar data more than once.
- Manuscript should complement any figures or tables, not duplicate the identical information.
- Never confuse figures with tables - there is a difference.

Approach

- As forever, use past tense when you submit to your results, and put the whole thing in a reasonable order.
- Put figures and tables, appropriately numbered, in order at the end of the report
- If you desire, you may place your figures and tables properly within the text of your results part.

Figures and tables

- If you put figures and tables at the end of the details, make certain that they are visibly distinguished from any attach appendix materials, such as raw facts
- Despite of position, each figure must be numbered one after the other and complete with subtitle
- In spite of position, each table must be titled, numbered one after the other and complete with heading
- All figure and table must be adequately complete that it could situate on its own, divide from text

Discussion:

The Discussion is expected the trickiest segment to write and describe. A lot of papers submitted for journal are discarded based on problems with the Discussion. There is no head of state for how long a argument should be. Position your understanding of the outcome visibly to lead the reviewer through your conclusions, and then finish the paper with a summing up of the implication of the study. The purpose here is to offer an understanding of your results and hold up for all of your conclusions, using facts from your research and generally accepted information, if suitable. The implication of result should be visibly described. Infer your data in the conversation in suitable depth. This means that when you clarify an observable fact you must explain mechanisms that may account for the observation. If your results vary from your prospect, make clear why that may have happened. If your results agree, then explain the theory that the proof supported. It is never suitable to just state that the data approved with prospect, and let it drop at that.

- Make a decision if each premise is supported, discarded, or if you cannot make a conclusion with assurance. Do not just dismiss a study or part of a study as "uncertain."
- Research papers are not acknowledged if the work is imperfect. Draw what conclusions you can based upon the results that you have, and take care of the study as a finished work
- You may propose future guidelines, such as how the experiment might be personalized to accomplish a new idea.
- Give details all of your remarks as much as possible, focus on mechanisms.
- Make a decision if the tentative design sufficiently addressed the theory, and whether or not it was correctly restricted.
- Try to present substitute explanations if sensible alternatives be present.
- One research will not counter an overall question, so maintain the large picture in mind, where do you go next? The best studies unlock new avenues of study. What questions remain?
- Recommendations for detailed papers will offer supplementary suggestions.

Approach:

- When you refer to information, differentiate data generated by your own studies from available information
- Submit to work done by specific persons (including you) in past tense.
- Submit to generally acknowledged facts and main beliefs in present tense.

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Topics	Grades		
	A-B	**C-D**	**E-F**
Abstract	Clear and concise with appropriate content, Correct format. 200 words or below	Unclear summary and no specific data, Incorrect form Above 200 words	No specific data with ambiguous information Above 250 words
Introduction	Containing all background details with clear goal and appropriate details, flow specification, no grammar and spelling mistake, well organized sentence and paragraph, reference cited	Unclear and confusing data, appropriate format, grammar and spelling errors with unorganized matter	Out of place depth and content, hazy format
Methods and Procedures	Clear and to the point with well arranged paragraph, precision and accuracy of facts and figures, well organized subheads	Difficult to comprehend with embarrassed text, too much explanation but completed	Incorrect and unorganized structure with hazy meaning
Result	Well organized, Clear and specific, Correct units with precision, correct data, well structuring of paragraph, no grammar and spelling mistake	Complete and embarrassed text, difficult to comprehend	Irregular format with wrong facts and figures
Discussion	Well organized, meaningful specification, sound conclusion, logical and concise explanation, highly structured paragraph reference cited	Wordy, unclear conclusion, spurious	Conclusion is not cited, unorganized, difficult to comprehend
References	Complete and correct format, well organized	Beside the point, Incomplete	Wrong format and structuring

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ISSN 9755896