On the
Non-Linearity of Diffuse Reflection 'Absorbance' Spectra of Skin

Summary: The -log(R_{diff}) 'absorbance' spectrum of skin is non-linear in the absorption coefficient μ_a of the tissue. This report is based on the conclusions made in my report on "The Effects of Biological Variability on the -log(R) Spectra of Skin" dated 14-Dec-1993; where a general description of the phenomenon was provided. This report contains quantitative estimates of the effects in skin.

Lambert-Beer does not hold for diffuse reflection experiments. The amount of non-linearity is dependent on the scatter characteristics μ_s, g of the probe, i.e., the probability distribution of the pathlength which a photon would travel thru the skin before escaping the *non*-absorbing tissue (at μ_a=0 every photon will finally leave the skin). The distribution of this "photon pathlength" $p_\#(l)$ was estimated using Monte-Carlo simulations and was found to be approximated by a log-normal distribution. This is in compliance with theory requiring non-negative physical variables to be log-normally distributed in a state of maximum entropy.[1] The non-linear dependence of the output signal -$\log_{10}(R_{diff})$ on the tissue absorbance coefficient μ_a, is given by:

$$-\log_{10}\bar{R}_{diff} = -\log_{10}\left(\int_0^\infty p_\#(l)\ e^{-\mu_a l}\, dl\right) \qquad (1)$$

and is documented in Figs.1 and 2 where the tissue operating points at different wavelengths are marked "★." Since the mean "photon pathlength" thru skin ranges between ca. 29-57 mm in the near IR and is much larger than the average pathlength of the diffusely reflected *power*, significant deviations from the Lambert-Beer Law result.[2] Fig.2 show first-order derivatives of Fig.1 which may be interpreted as the effective pathlength of the diffuse reflection 'cuvette' at a given value of μ_a (non-linearity) for a particular value of μ_s (instationarity).
The **non-linearity is severe especially in the main glucose region** around λ=1570 nm where the effective 'cuvette' pathlength changes with μ_a at a rate of roughly -1%/%. The effective pathlength at λ=1570 nm, is about *3x* larger than it is at the water absorbance peak around λ=1430 nm.

Conclusion: Biological and sampling variabilities result is significant *multiplicative* calibration errors that can not be handled by usual PLS or other linear calibration algorithms. Stated positively: significant improvements can be expected from the development of calibration algorithms that do account for diffuse reflection non-linearity. These algorithms will need to find an appropiate multiplicative correction factor that is determined from and applied to, the measured -log(R_{diff}) spectrum. Standardizing the calibration spectra to equal height, e.g., of a water absorption peak, is not sufficient.

This is a mistake, The model is in essence, NOT an algorithm. But in general, this conclusion is TRUE!

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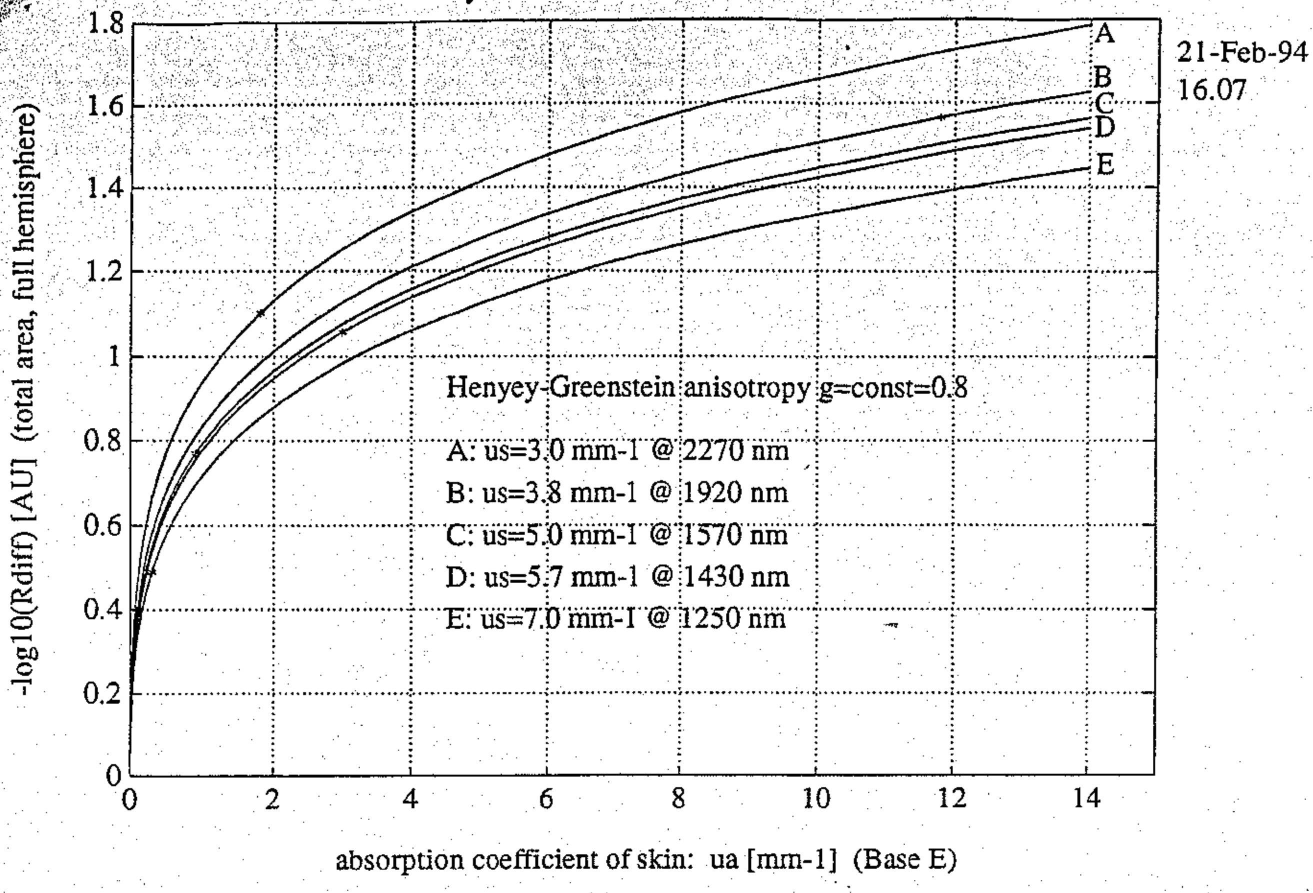
1. A. Tarantola, "Inverse Problem Theory," Amsterdam: Elsevier, 1987; p. 22 ff.

2. The results of the Monte-Carlo simulations as well as further details of the log-normal fit, will be presented in my forthcoming memo on "Biological and Sampling Variations."

Non-Linearity of Diffuse Reflection 'Absorbance' Signal



ZOOM of above

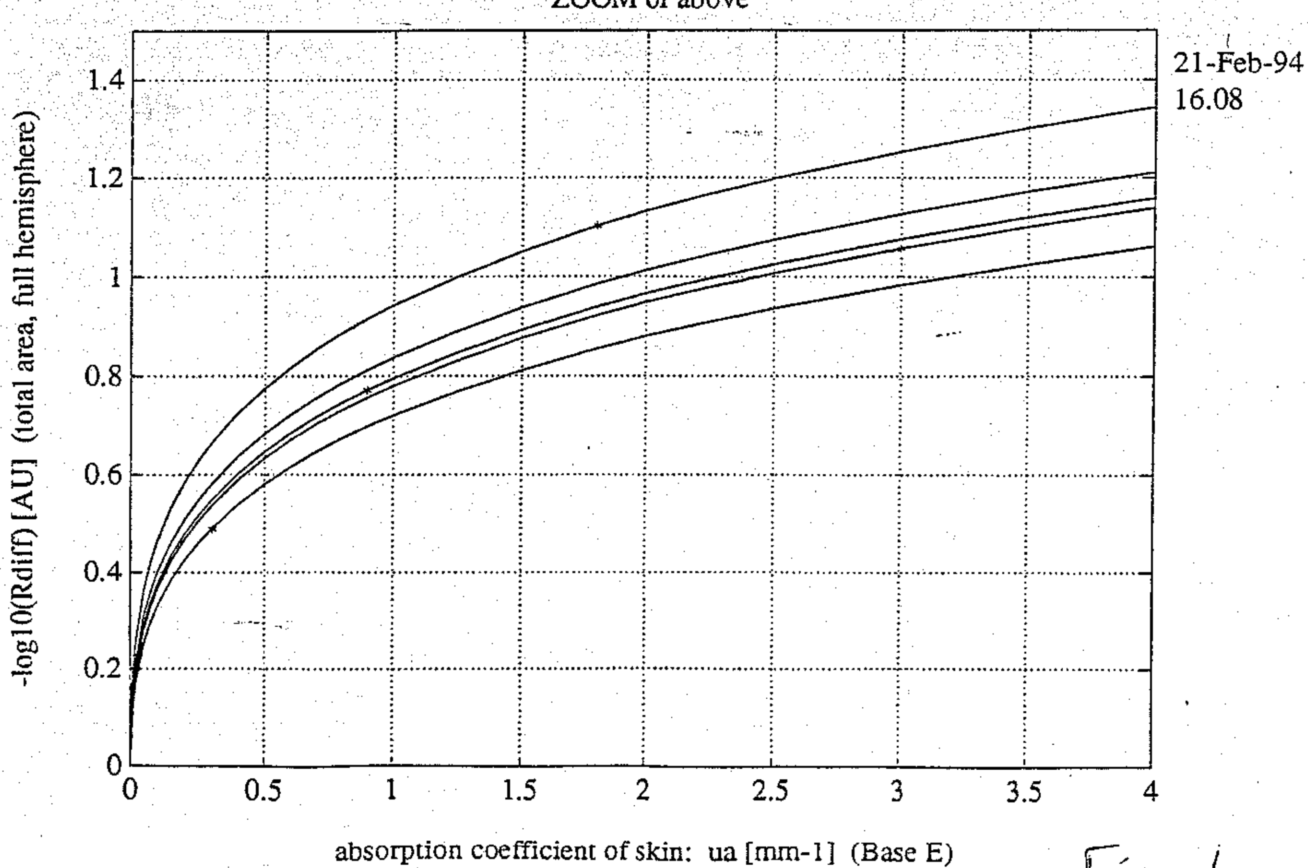
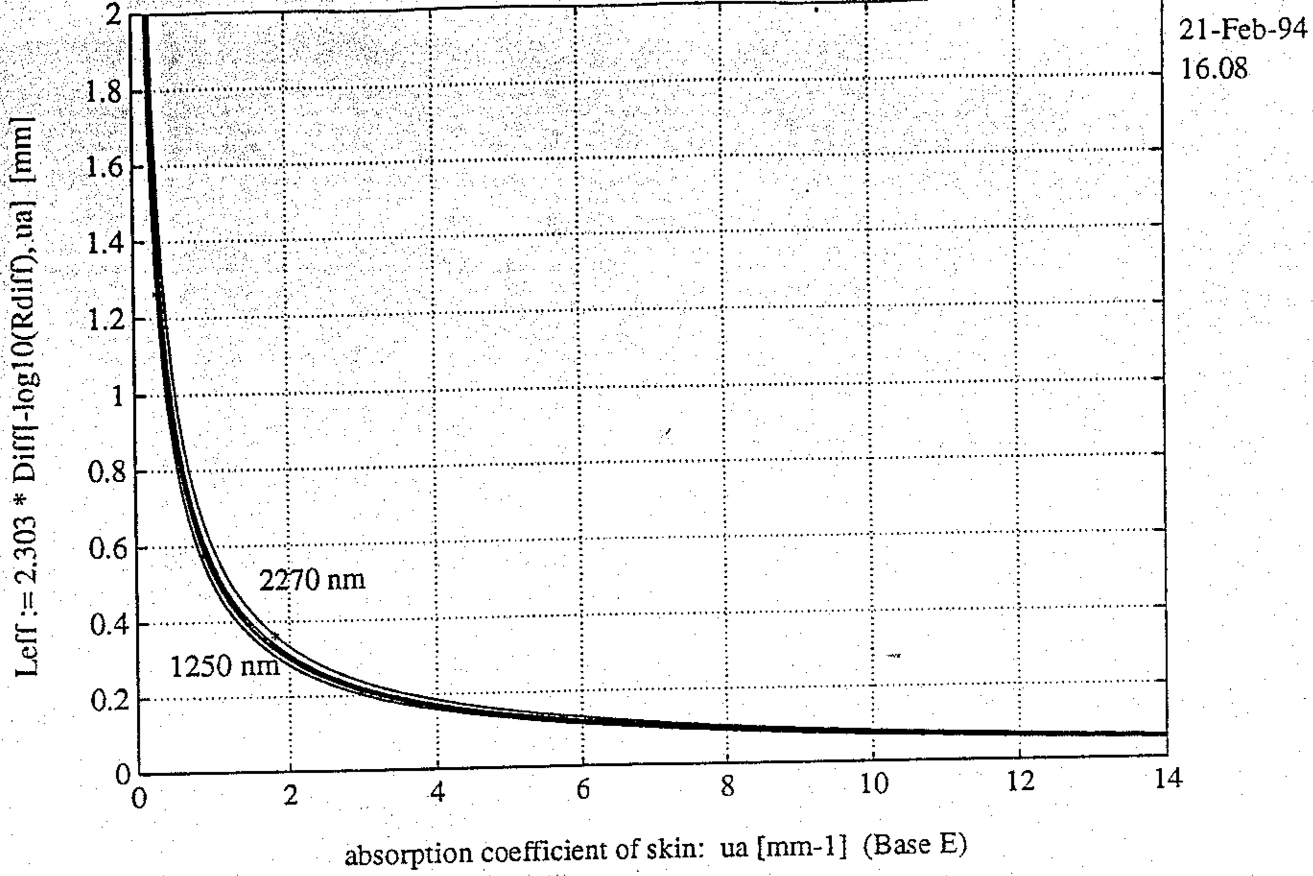


Fig. 1



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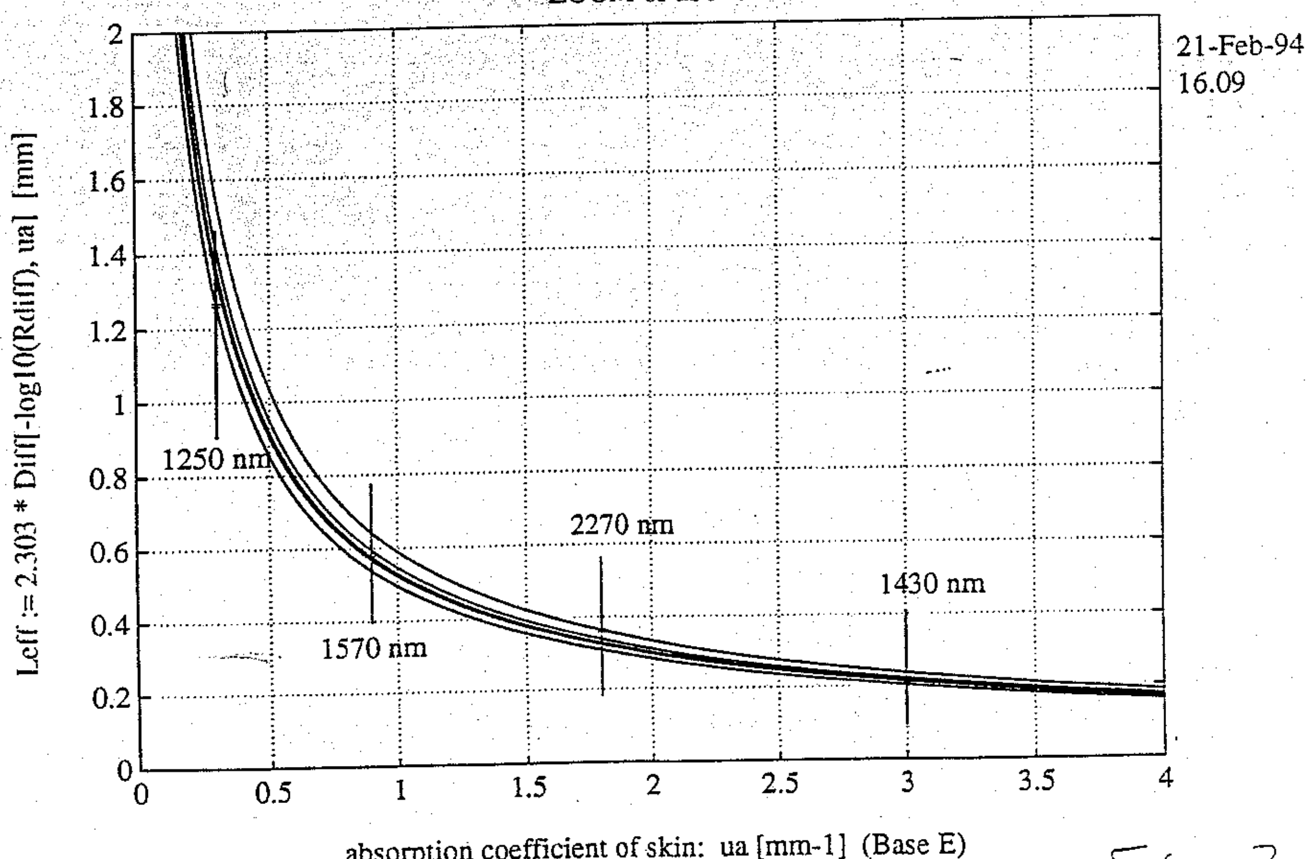


Fig. 2

Note on

POSSIBLE CURE FOR R_{diff} - Nonlinearity

Scenario of DIFFUSION THEORY:

- a semi-infinite turbid medium is illuminated with an ideally diffuse beam of light, i.e., the incident, reflected, and transmitted (if any) light are all Lambertian
- the Lambertian differential absorption and scattering coefficients at a given wavelength, are W and K [m^{-1}], respectively (Kubelka-Munk theory)

⇒ the total diffuse reflectance R (w/o Fresnel-reflection and integrated over the whole hemispherical solid angle and area) is:

$$R = \frac{K}{W + K + \sqrt{W(2K+W)}}$$

$W \propto \mu_a$ ... tissue absorption coefficient

$K = \text{function}(\mu_s, g)$

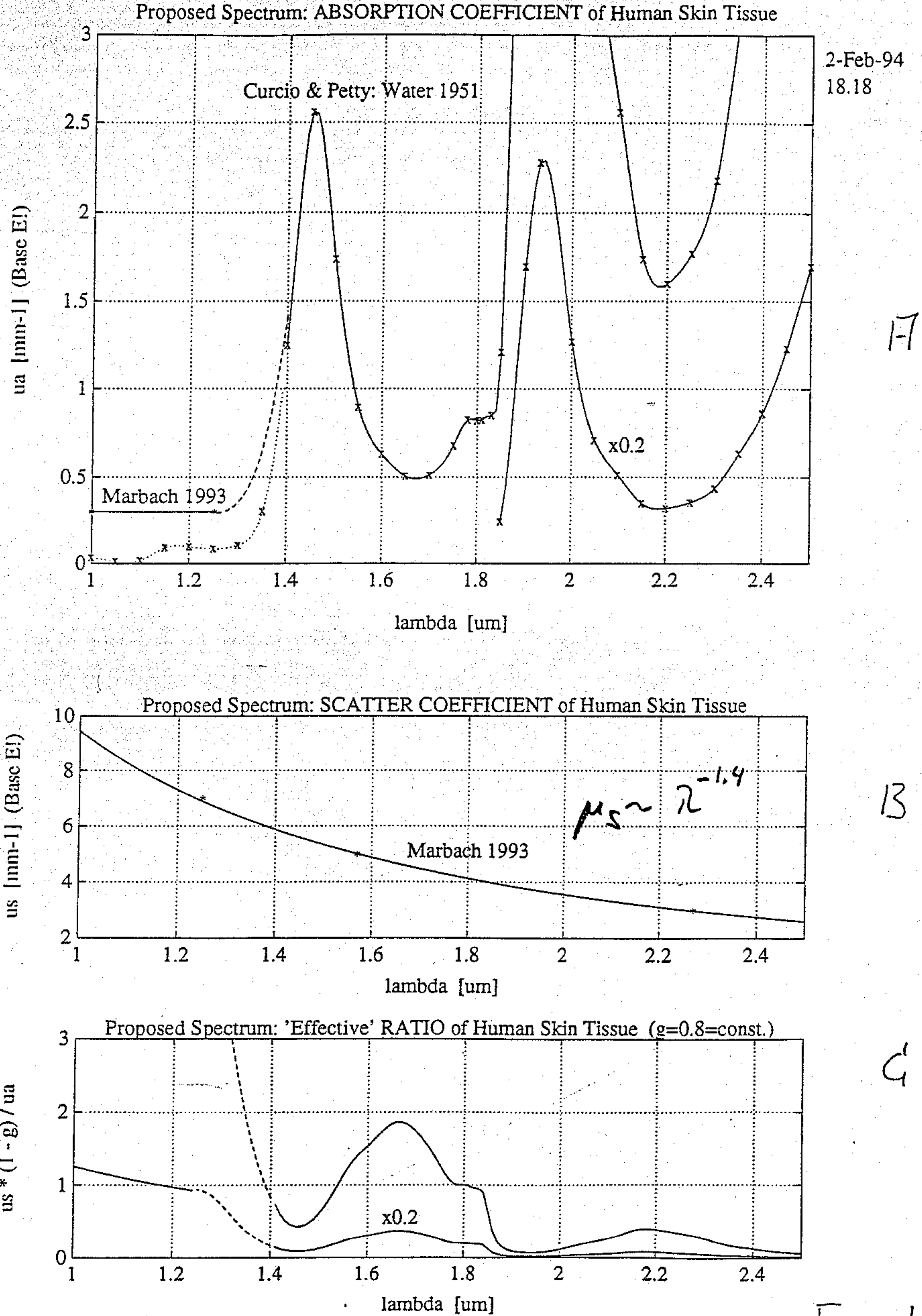
tissue scattering characteristics

use as start values:

$$W = 2\mu_a$$

$$K = \frac{3\mu_s(1-g) - \mu_a}{4}$$

Cheong et al., "Review of Optical Properties of Biological Tissues," IEEE J. Quantum Electron., 26, 2166 (1990



Proposed Spectrum: ABSORPTION COEFFICIENT of Human Skin Tissue
2-Feb-94
18.18
Curcio & Petty: Water 1951
Marbach 1993
x0.2
ua [mm-1] (Base E!)
lambda [um]
17
Proposed Spectrum: SCATTER COEFFICIENT of Human Skin Tissue
Marbach 1993
$\mu_s \sim \lambda^{-1.4}$
us [mm-1] (Base E!)
lambda [um]
13
Proposed Spectrum: 'Effective' RATIO of Human Skin Tissue (g=0.8=const.)
x0.2
us * (1 - g) / ua
lambda [um]
G

Fig. 1

Monte-Carlo Simulation of Diffuse Reflection of Skin in the Near-Infrared Spectral Range. *μ_a, μ_s, g, n the absorption* and scattering coefficient (base E), the anisotropy, and the refractive index of skin, respectively. R_{diff} is the *total* diffuse reflection of the radiation power integrated over infinite area and full hemisphere; the total reflected power is distributed over: **r** the radial distance between entrance and exit points; $\mathbf{z_{max}}$ the maximum penetration depth reached into the skintissue; $\mathbf{z_{av}}$ the mean penetration depth; and **L** the total pathlength through the tissue; the mean values of these distributions are given in the table. ($\mathbf{R_\#}$ is a software parameter providing the additional information of what fraction of the photons were actually re-emitted in the simulation runs before loosing 99.95% of their power.)
$L_\#$ is the mean distance a photon would travel thru the tissue if the skin were non-absorbing (μ_a=0). The probability distribution of this pathlength can be approximated by a log-normal distribution the mean and standard deviation of which are given in the last two columns of the table.[1]

Simulation Parameters					Power Statistics						Photon Escape Ststcs (μ_a=0)		
												$x:=\log_e(L_\#/mm)$	
λ [μm]	μ_a [mm^{-1}]	μ_s [mm^{-1}]	g	n	r [mm]	z_{av} [mm]	z_{max} [mm]	L [mm]	$R_\#$	R_{diff}	$L_\#$ [mm]	E[x]	Std[x]
1.25	0.3	7.0	0.8	1.37	0.3442	0.2731	0.5013	1.9911	0.72648	0.27409	29.295	2.0027	2.5445
	-1%				0.34%	0.68%	0.71%	0.88%	0.23%	0.41%	-	-	-
		+1%			-0.85%	-0.48%	-0.49%	-0.36%	0.27%	0.69%	1.60%	-0.68%	-
1.43	3.0	5.7	0.8	1.37	0.1231	0.0584	0.1111	0.3568	0.23755	0.02927	44.653	2.2742	2.7672
	-1%				0.59%	1.18%	1.13%	1.15%	1.00%	1.35%	-	-	-
		+1%			-0.42%	-0.05%	-0.09%	-0.05%	0.97%	1.37%	-2.33%	-1.48%	-
1.57	0.9	5.0	0.8	1.37	0.2655	0.1643	0.3061	1.0606	0.47852	0.08694	46.916	2.3417	2.5576
	-1%				0.55%	0.73%	0.68%	0.82%	0.32%	1.01%	-	-	-
		+1%			-0.45%	-0.12%	-0.14%	-0.12%	0.66%	1.20%	-1.92%	-0.35%	-
1.92	11.8	3.8	0.8	1.36	0.0406	0.0146	0.0283	0.0854	0.03768	0.00462	47.834	2.5189	2.5510
	-1%				1.35%	1.34%	1.36%	1.37%	1.00%	0.94%	-	-	-
		+1%			-0.14%	0.10%	0.10%	0.01%	0.82%	0.98%	1.15%	0.03%	-
2.27	1.8	3.0	0.8	1.34	0.2131	0.0988	0.1883	0.5998	0.20962	0.02596	56.968	2.9442	2.8493
	-1%				0.36%	0.57%	0.53%	0.61%	0.91%	1.35%	-	-	-
		+1%			0.01%	-0.02%	-0.05%	0.15%	1.14%	0.95%	-0.62	-0.35%	-

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The results r, z_{av}, z_{max}, L, and R_{diff} are statistically significant to about two decimal places (averages of 5000 diffusely reflected photons); the precision of the sensitivity numbers is the relative precision of the results, i.e., about one decimal place. $L_\#$, $E[\ln(L_\#)]$, and $Std[\ln(L_\#)]$ are averaged over 500 photons only.

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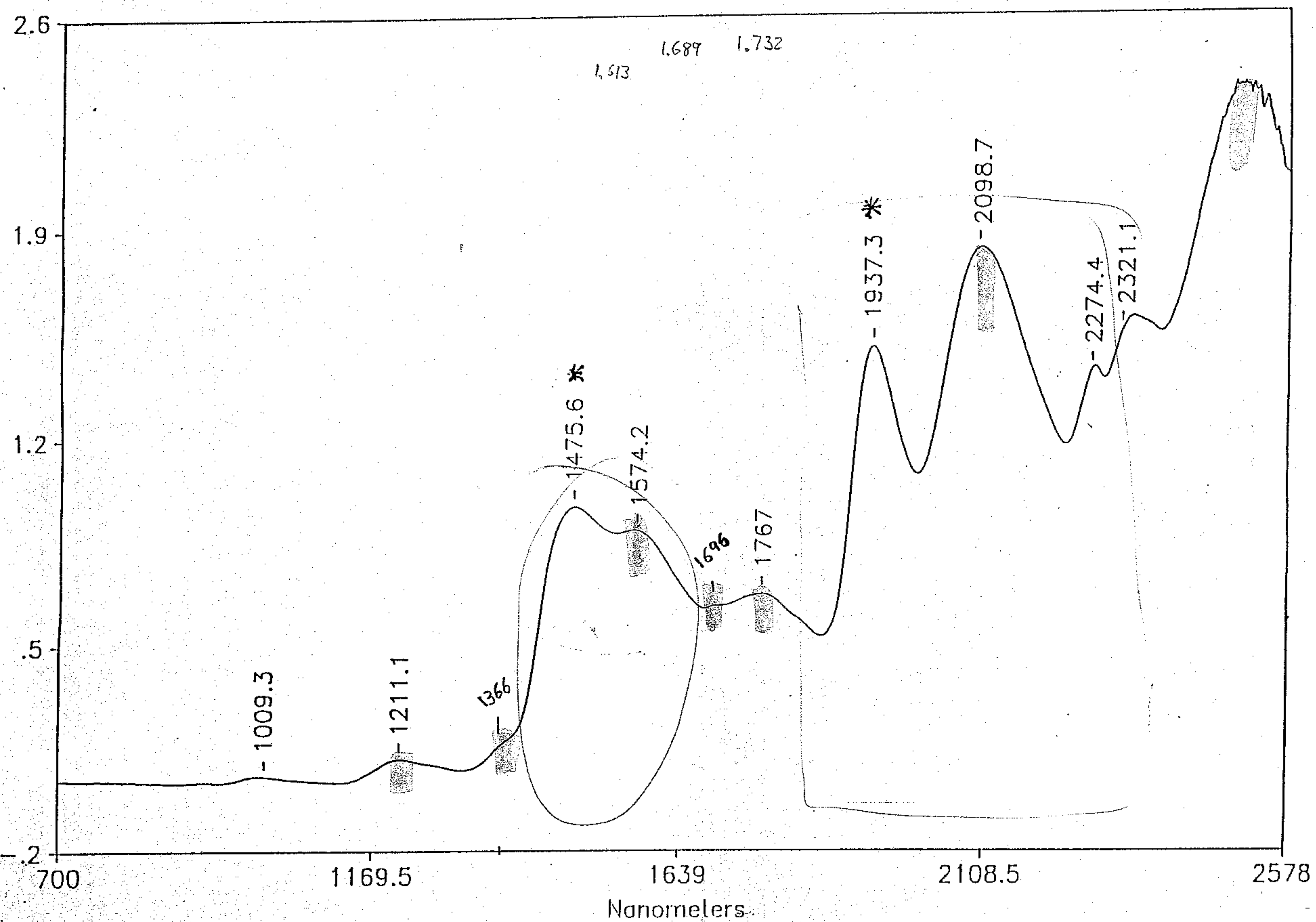
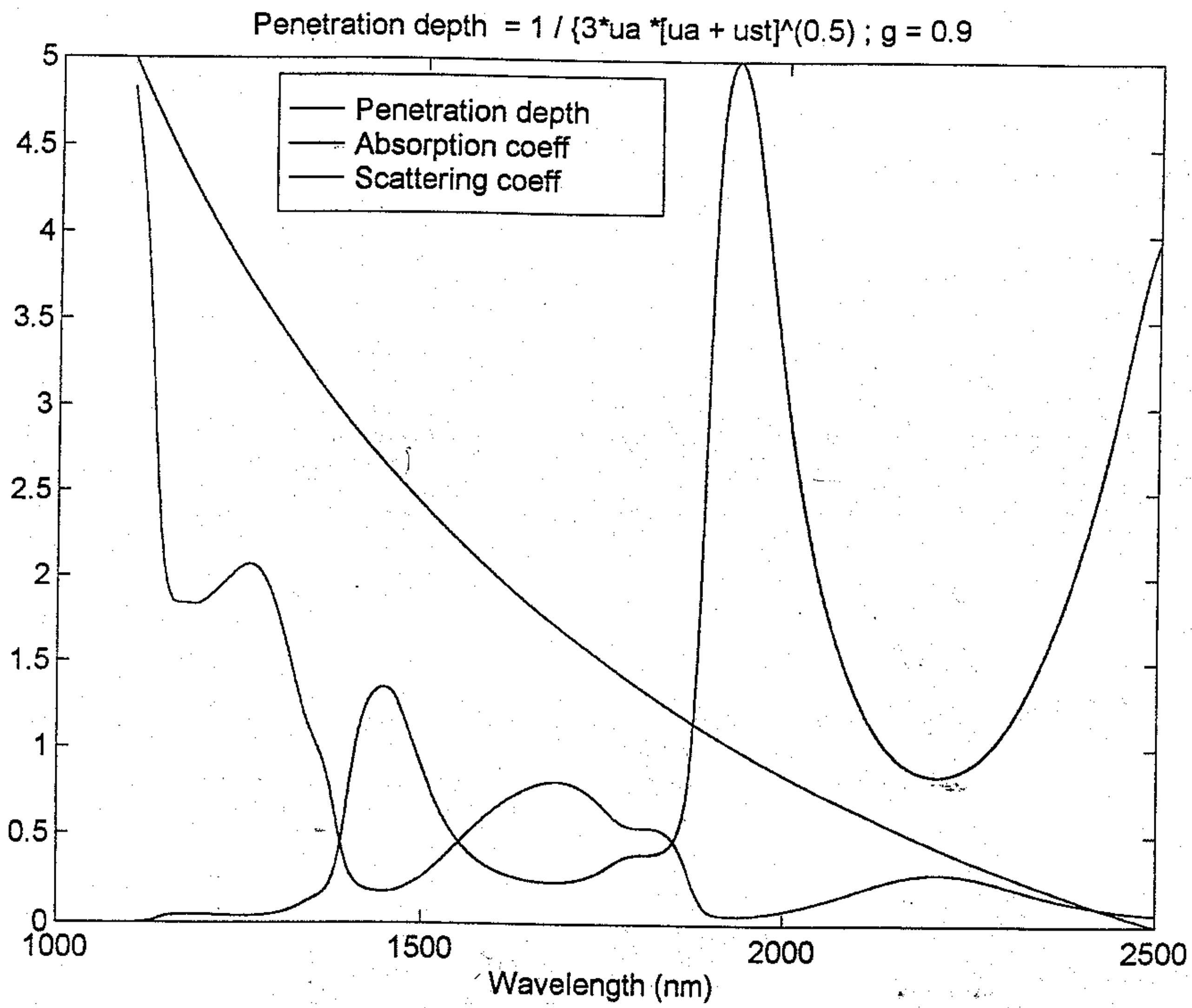
Amorphous Glucose Spectrum Provided by Karl Norris



transmittance measures


Penetration depth = 1 / {3*ua *[ua + ust]^(0.5) ; g = 0.9
Penetration depth
Absorption coeff
Scattering coeff
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5
1000
1500
2000
2500
Wavelength (nm)