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COMPUTATIONAL METHODS FOR THE DESIGN OF TEST OBJECTS AND TISSUE SUBSTITUTES FOR RADIOLOGIC APPLICATIONS

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Abstract — A theoretical framework has been developed for the design of tissue substitutes for use with diagnostic X rays. The theory divides naturally into a three-level hierarchy in which the number of properties of a reference material that can be matched by a substitute material increases with the number of components used in the substitute material. For a single component, the thickness can be chosen so as to match transmitted spectral shape or overall attenuation of the reference material, but not both. Two components can be combined to match both the spectral shape and overall attenuation, but not the thickness of a reference object. Use of three components permits matching of the spectral shape, overall attenuation, and thickness of the reference object, i.e. the linear attenuation coefficient of the substitute material matches that of the reference material. Examples are presented, and the theory is compared with other, similar methods.

INTRODUCTION

Since the only practical source of X rays for medical radiography is the X ray tube, which generates a highly polyenergetic spectrum, tissue substitutes should provide accurate simulation over a broad range of energies. The energy range considered here is 10 to 150 keV. Qualitative arguments indicate that when the overall attenuation of a test object matches that of the reference material over a large energy range, the magnitudes of photoelectric and Compton interactions will also be reasonably well matched to those of the reference material. Thus the approach taken here is to study algorithms based on total coefficients and simply examine the partial coefficient fits for suitability.

THEORY AND NUMERICAL IMPLEMENTATION

Single-component simulations

With a single material, it is possible to find a thickness that will match either the quantity or the quality of radiation transmitted by a reference object. In the case of a single photon energy, the condition for matching the quantity of radiation is that the transmissions be equal at the energy of interest, which leads to the relation

$$\mu_0 t_0 = \mu_1 t_1 \qquad (1)$$

where μ is linear attenuation coefficient, t is thickness, and subscripts 0 and 1 refer to the reference material and substitute material, respectively. When a spectrum Φ is involved, the energy response of the detector, $R_D(E)$ must be taken into account since 'quantity of radiation' only has meaning in terms of the effect it produces, as, for example, in an ionisation chamber or intensifying screen. Thus the condition is that the integrals of the transmitted spectra for the reference object and the substitute, weighted by the detector response, be equal, or

$$\int \Phi(E)\exp(-\mu_0(E)t_0)R_D(E)dE = \int \Phi(E)\exp(-\mu_1(E)t_1)R_D(E)dE \qquad (2)$$

This condition has considerable practical importance, and a numerical algorithm has been developed that solves Equation 2 for t_1. Since Equation 2 ignores scattered radiation, the solutions are only valid for cases where scatter is eliminated (narrow beam geometry, or with a perfect grid), or where the reference and substitute materials generate similar scatter fields. In other situations, more rigorous methods, such as the Monte Carlo calculations reported by Carrier and Blais[1] and by Sandborg *et al*[2], must be used.

To match the quality of the radiation, i.e. spectral shape, transmitted by a reference object, the transmission of the substitute material must be a constant fraction of the transmission of the reference object over the relevant range of energies. This condition can be written

$$\exp(\mu_1 t_1 - \mu_0 t_0) = r \qquad (3)$$

where r is independent of energy for at least some small range of energies. Taking the natural logarithm and energy derivative of both sides and imposing the condition that dr/dE = 0 yields

$$\mu_0' t_0 = \mu_1' t_1 \quad (4)$$

where $\mu_i' \equiv d\mu_i/dE$. The thickness of test material that provides a spectral match to the reference material is thus given by

$$t_1/t_0 = \mu_0'/\mu_1' \quad (5)$$

Although the ratio of derivatives in Equation 5 is not independent of energy, as would be required for a perfect match, it is still possible to find a single thickness ratio that provides a good spectral match. An analysis of this observation has been presented previously[3]. The point that is important for the theoretical development that follows is that a reasonably accurate spectral match is possible over a large range of energies.

Two-component simulations

The following theoretical development is similar to one presented previously[4]. Spectrally accurate phantoms that also transmit the correct quantity of radiation must satisfy two conditions, Equations 1 and 4. In general, both equations cannot be satisfied simultaneously by a single material. However, if there is a substitute material that, when spectrally matched to the reference material transmits more than the reference material, and there is a second that transmits less, a combination of the two can be found that produces the same spectral shape as well as the same transmission as the reference material. Allowing two components for the substitute material in Equations 1 and 4 gives a set of two equations in two unknowns, with the following solution:

$$a_1 = t_1/t_0 = (\mu_0\mu_2' - \mu_2\mu_o')/(\mu_1\mu_2' - \mu_2\mu_1')$$

$$a_2 = t_2/t_0 = -(\mu_0\mu_1' - \mu_1\mu_o')/(\mu_1\mu_2' - \mu_2\mu_1') \quad (6)$$

In general $a_1 + a_2 \neq 1$.

The simulation provided by Equations 6 is exact only if a_1 and a_2 are independent of the energy at which the attenuation coefficients and their derivatives are evaluated. Since such independence is never exact, the following algorithm has been developed. First, an energy array is established based on user specified values of minimum energy, energy increment, and maximum energy. For the materials selected, attenuation coefficients are then generated at every point in the energy array using polynomial fits for the coefficients provided in the compilation of tabulated data of McMaster *et al*[5]. Derivatives are obtained by straightforward differentiation of the polynomials. Next, relative thickness pairs (a_1,a_2) for the components of the substitute are calculated at each energy, using Equations 6. Finally, for the range of energies specified, the RMS error between the linear coefficient of the reference material and the 'effective' linear coefficient of the substitute is calculated for each pair of relative thicknesses. (Since equal transmission is the desired condition, μ_0 is to be compared to the 'effective' coefficient of the substitute, μ_{eff}, which is equal to $(a_1\mu_1 + a_2\mu_2)$, rather than the true linear coefficient of the substitute, $\mu_{eff}/(a_1 + a_2)$.) The pair giving the smallest error, and the corresponding linear coefficients and 'total scatter' coefficients (sum of Compton and coherent) for the substitute, are saved. Although the best pair is selected from the set of thicknesses (a_1,a_2) obtained by evaluating Equations 6 on the specified energy grid, the set does not necessarily contain the best pair that exists, so the algorithm is only quasi-optimal.

An example is the use of ethanol and glycol to simulate 50% glandular and 50% adipose, by weight, breast tissue. The elemental composition and density of the breast tissue are taken from the work of Hammerstein *et al*[6] (H, 0.107; C, 0.4015; N, 0.0245; O, 0.464; P, 0.003; specific gravity, 0.982 $g.cm^{-3}$). The energy range was 10 to 150 keV, with step size 1 keV. The algorithm yields relative thicknesses of 0.1091 and 0.8129, respectively, so that the relative thickness of the simulation material is 0.922. Ratios of linear and 'total scatter' coefficients, adjusted for the thickness difference, are plotted in Figure 1. The error in the 'effective' attenuation coefficient of the substitute material is less than 0.2% over the entire energy range considered. A similar example is the simulation of the same tissue by ethanol and water. The resulting

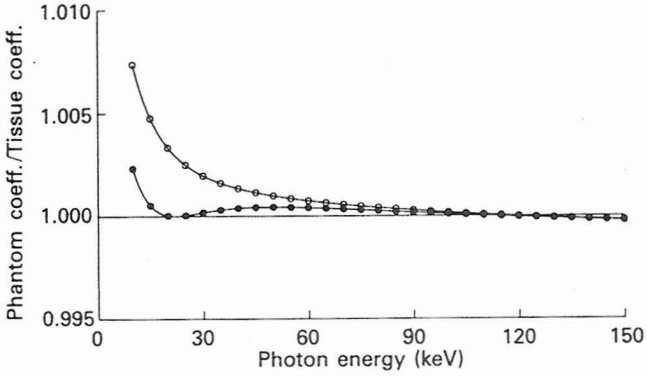

Figure 1. Ratios of linear attenuation coefficients (solid circles) and 'total scatter' (Compton plus coherent) coefficients (open circles) for the combination of ethanol and glycol calculated to simulate 50% glandular and 50% adipose breast tissue, and the corresponding coefficients for breast tissue.

relative thicknesses are 0.7994 and 0.3356, respectively, yielding a total relative thickness of 1.135.

The accuracy of these simulations is directly related to the fact, demonstrated by Alvarez and Macovski[7] and further elucidated by the work of Weaver and Huddleston[8], that only two independent functions are required to describe accurately the energy dependence of the total (narrow beam) attenuation coefficient of any material of biological interest at energies in the diagnostic X ray energy range. One possible choice of the two functions is closely related to the fundamental interactions involved. They are the functions that describe photoelectric absorption and Compton scattering. The contribution of coherent scattering to the total attenuation coefficient is, to a certain extent, representable by a combination of these functions[9]. The procedure used here to select amounts of the two phantom components has thus yielded a combination such that the sum of the photoelectric contributions and the sum of the Compton contributions are approximately equal to the photoelectric and Compton components, respectively, of the total attenuation coefficient of the reference material. The close agreement of 'total scatter' coefficients (open circles, Figure 1) supports this.

The notion that the same two functions can describe every material of interest leads naturally to a two-energy formulation of the problem[7]. In this formulation two equations, both of the form $\mu_0(E)t_0 = \mu_1(E)t_1 + \mu_2(E)t_2$ but with different values of energy E, are to be solved. The solutions are

$$a_1 = (\mu_{01}\mu_{22} - \mu_{21}\mu_{02})/(\mu_{11}\mu_{22} - \mu_{21}\mu_{12})$$
$$a_2 = -(\mu_{01}\mu_{12} - \mu_{11}\mu_{02})/(\mu_{11}\mu_{22} - \mu_{21}\mu_{12}) \quad (7)$$

where $\mu_{ij} \equiv \mu_i(E_j)$.

An algorithm that calculates relative thickness pairs (a_1,a_2) for all possible combinations of energies (as opposed to permutations) in the array specified by the user, and is otherwise similar to the one described above, has been implemented for the two-energy approach. It is useful in designing two-component phantoms from measured transmission data. In this application, values of the product $\mu_0 t_0$ for the reference object are replaced by values of $\ln(n_i/n_t)$, where n_i and n_t are incident and transmitted photon counts at a given energy, obtained by X ray spectroscopy. Since there are statistical fluctuations in the transmission data from one energy to the next, numerical differentiation of such data would introduce large errors, and smoothing of the data by curve fitting might introduce biases. Use of the algorithm based on the two-energy formulation of the problem avoids these difficulties. While the calculations suggest that good simulation properties can be obtained with two-component phantoms, many additional steps are involved in the development of a satisfactory attenuation phantom, and in the verification of its patient equivalence[10].

Three-component simulations

As noted above, two-component phantoms do not, in general, match the thickness of the object being simulated, so a third condition, which specifies the thickness of the substitute relative to the reference material, is required. Since in working with liquids it is necessary to compensate for the volume changes that occur on mixing, and because of interest in materials that have CT contrast that is independent of energy, the thickness matching requirement can be generalised to one of linear proportionality by requiring that the thickness of the phantom be equal to the thickness of the reference object multiplied by a constant. Imposing a third condition requires that a third phantom component be allowed, so the thickness matching equation is

$$kt_0 = t_1 + t_2 + t_3 \quad (8)$$

The solution of the set of three equations formed by Equation 8 and the three-component versions of Equations 1 and 4 is

$$a_1 = [\mu_2'(\mu_0 - k\mu_3) + \mu_3'(k\mu_2 - \mu_0) + \mu_0'(\mu_3 - \mu_2)]/D$$
$$a_2 = [\mu_3'(\mu_0 - k\mu_1) + \mu_1'(k\mu_3 - \mu_0) + \mu_0'(\mu_1 - \mu_3)]/D$$
$$a_3 = [\mu_1'(\mu_0 - k\mu_2) + \mu_2'(k\mu_1 - \mu_0) + \mu_0'(\mu_2 - \mu_1)]/D \quad (9)$$

where $D = \mu_1'(\mu_3 - \mu_2) + \mu_2'(\mu_1 - \mu_3) + \mu_3'(\mu_2 - \mu_1)$.

A straightforward extension of the algorithm developed to implement the solution to the two-component, derivative-based formulation of the tissue simulation problem has been developed for the three-component case. It has been applied to the simulation of 50/50 breast tissue by ethanol, glycol and water, with the thickness ratio k set to unity, and the energy range as specified for the two-component simulations. The solution is $(a_1,a_2, a_3 = 0.3616, 0.5163, 0.1221)$. Note that a_1, a_2, and a_3, being relative thicknesses, should be treated as fractions by volume, not mass. Total and partial coefficient ratios for this simulation are shown in Figure 2. The errors in the photoelectric and

coherent coefficients offset each other, leading to the good agreement in total coefficient data. Possible approaches for improving the agreement of partial coefficients, both of which are suggested by the work of Geske[11,12], include use of a figure of merit based on partial as well as total coefficients, and use of an additional equation based on either the coherent or photoelectric partial coefficient.

Because of the change in the total volume of the liquids used in this simulation when they are mixed, the values for a_1, a_2 and a_3 obtained with k = 1.00 do not produce the desired match to breast tissue volume. To correct for the volume change, an iterative approach can be used. Since in this case volume decreases, a value of k slightly greater than 1.00 is specified, the three phantom components are mixed in ratios corresponding to that value of k, and the resulting volume is measured. These steps are repeated until the desired final volume is obtained. A similar approach has been described by Geske[12].

The simulation of 50% glandular and 50% adipose breast tissue has been repeated with varying values of k to find solutions for the range of relative thickness that corresponds to non-negative thicknesses of the phantom components. The volume fractions of the three components are plotted as a function of k in Figure 3. The k values correspond to the total volume of the phantom constituents, relative to breast tissue, before mixing. The volumes of the two components that remain when the calculated solution requires a zero thickness of the third component are exactly the values of a_1 and a_2 calculated by the two-component algorithm.

Comparison of simulation methods

The method for designing three-component tissue simulating materials described above is similar to methods described by White[13], Geske[11,12] and Hermann *et al*[14,15]. Although additional analytic procedures, including the *elemental equivalence* procedure, the *effective atomic number* procedure, and the related *extended $\bar{Y}$ method* are also of interest, they have been described in the review by White[16], and will not be discussed here.

The *basic data method* of White[13] requires that two equations be satisfied. One involves the magnitude of the interaction effect of interest for the tissue being simulated and the substitute at a given energy, and is analogous to Equation 1 above. The other requires equality of the relative masses of the tissue and simulation material, and is analogous to Equation 8 above. (Tissue simulation problems can, in general, be stated in terms of either linear or mass coefficients. The relationship between the two formulations is given by Geske[11].) Although not listed explicitly, a third equation, which is related to Equation 4, is implied by the fact that the quality of the simulation yielded by the two equations is determined based on the deviation of the parameter of interest at other energies. In fact, the system implemented by White specifies the required radiation properties of a filler material for a given primary material so that a data base can be searched for the most suitable choice of filler. The *basic data method* is considerably more general than the method discussed here since it deals with particle and high energy photon interactions as well as both partial and total photon coefficients in the diagnostic energy range.

The papers by Geske[11,12] consider a wide variety of analytic approaches, including ones not discussed here, to the simulation of the interaction properties of tissue with radiation. The most directly related approach involves matching of tissue and substitute attenuation coefficients at suitable energies, and equality of thickness or mass, depending on whether

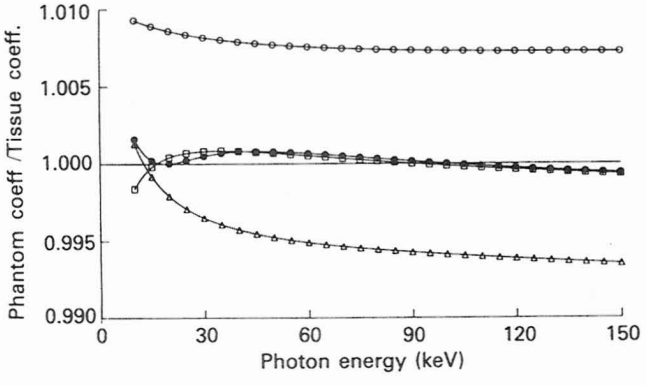

Figure 2. Ratios of total and partial attenuation coefficients for the simulation of 50% glandular and 50% adipose breast tissue by ethanol, glycol, and water. Errors in photoelectric and coherent coefficients offset each other. (●) total, (○) coherent, (□) Compton, (△) photoelectric.

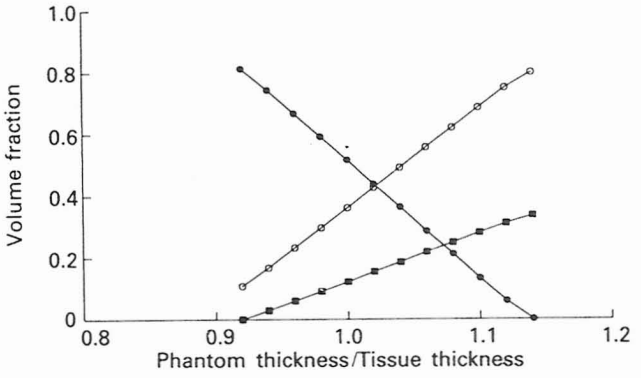

Figure 3. Relative volumes of ethanol (○), glycol (●) and water (■) required to simulate 50% glandular and 50% adipose breast tissue as a function of k, the ratio of the overall volume of the phantom components, before mixing, to the tissue volume.

the linear or mass attenuation coefficient is being simulated. In the example cited by Geske, four energies, and hence five components, were used. The two-energy, two-component design procedure described above for attenuation phantoms, if supplemented by Equation 8, would constitute a limited case of Geske's more general approach. Another approach considered by Geske requires equality of various combinations of 'material parameters', specified as Z^n/A (Z is atomic number, A is relative atomic weight, and n = 1, 2, 4), and partial and total coefficients, at a single energy, along with mass or thickness. Although most of the examples given by Geske involve more than two parameters, the development above using total attenuation coefficients and their energy derivatives is similar in kind if it is considered that the equality of energy derivatives is equivalent to equality of some admixture of partial coefficients that is heavily weighted to the photoelectric coefficient when the derivatives are evaluated at low energies. The appeal of the energy derivative as a parameter is that it yields a substitute that not only matches the tissue being simulated, but also varies with energy at the same rate as the tissue being simulated, at the energy selected.

The method employed by Hermann *et al*[14,15] consists of the multi-energy, attenuation coefficient matching method given by Geske, but with only two energies, 10 and 150 keV. As mentioned in the discussion of Geske's methods, this approach is closely related to the two-energy, two-component system of equations described above. It is also related to the three-component, energy derivative formulation that has been described. If the attenuation coefficient derivatives that appear in the relative thickness solutions given in Equations 9 are expanded according to the mathematical definition of derivative, and the limits removed, the solutions to the corresponding two-energy statement of the three-component simulation problem are recovered. Such a procedure would be valid, i.e. the solutions would be independent of energy, only if the attenuation coefficients involved were all expressible as weighted sums of the same two energy functions. Since this is only approximately true, Hermann *et al* used an iterative adjustment procedure to find an optimal combination of two linearly independent combinations of components. This adjustment procedure has the advantage that it takes into account the non-calculable effects involved in the mixing of the phantom components.

CONCLUSIONS

Methods have been described for the design and evaluation of one-, two-, and three-component materials that have a variety of applications in diagnostic radiological physics. Comparison shows the methods to be conceptually related to a number of other techniques reported in the literature. The use of a figure of merit that evaluates the quality of a simulation everywhere in the energy region of interest provides a means of selecting the best of a number of possible solutions to a given simulation problem. The simulations that result are extremely accurate when the components of the substitute are appropriately chosen. The methods have been implemented in the form of FORTRAN programs for DOS-based personal computers.

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