Mathematical modelling of depth-dose response of polymer gel dosimeters

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Abstract. A dynamic partial differential equation (PDE) model is used to simulate the effects of radiation depth-doses on polymer formation in Polyacrylamide Gel (PAG) dosimeters. Depth-doses are simulated using different types of radiation including Co⁶⁰ gamma and 6 and 15 MV X-ray photon beams, along with 6, 9, 12, 16 and 20 MeV electron beams. Effects of monomer diffusion (edge enhancement) and temperature are studied. Diffusion results in excess polymer formation at the position of maximum dose (4% for Co⁶⁰ γ-radiation and less for other types of radiation studied). Temperature increases on the order of 2 °C increase the mass of polymer formed by approximately 2-3%. These results provide insight for calibrating dosimeters using depth-dose information.

1. Introduction
Polymer gel dosimetry is based on the dose dependant polymerization of monomers dispersed in an irradiated gel substrate. The polymerization is well behaved when the irradiation is essentially uniform. Measurements and modelling have shown that in non-uniform conditions with large dose gradients, such as the edge of a beam, the degree of polymerization at the edge of the irradiation may be enhanced by monomer diffusing from low dose areas (e.g., Fuxman et al. [1,2], Vergote et al. [3]). This has not been characterized in more gentle dose gradients. This article uses simulations to investigate the influence of depth-doses on the behaviour of PAG dosimeters. The primary objective is to predict the amount of polymer formed and the temperature at various depths in response to Co⁶⁰ γ-radiation, 6 and 15 MV X-ray photon beams, and 6 MeV to 20 MeV electron beams. Use of the model enables examination of monomer diffusion effects and temperature effects, which can influence the accuracy of dosimeter calibration using depth-dose information [4]. The current research focuses on 6%T 50%C PAG dosimeters containing 5% gelatin. Note that the model could also be used to simulate NIPAM-based dosimeters and PAG dosimeters with other recipes.

2. Materials and Methods
2.1. Primary Data for Depth-Doses
The percent depth-dose (PDD) data used in this study were from clinical measurements for various clinical radiation units. Clinical data under standard reference conditions (10 x 10 cm² field sizes at
standard source to surface distance) were taken for Co\textsuperscript{60} gamma and 6 and 15 MV X-ray photon beams (Fig. 1a), along with 6, 9, 12, 16 and 20 MeV electron beams (Fig. 1b).

Different cubic splines were used to convert the experimental depth-dose data for the various radiation beams in Fig. 1 to a convenient functional form for use in the PDE model. Additional spline nodes were used near the maxima of the PDD curves to ensure that accurate depth-dose information was provided to the model.

Figure 1. Percent depth-dose data by: (a) Co\textsuperscript{60} γ-radiation and 6 and 15 MV X-ray photon beams; (b) 6, 9, 12, 16 and 20 MeV electron beams.

2.2. Model Development

PDE material balances on chemical species in aqueous and polymer phases of PAG dosimeters were formulated by Fuxman et al. [1,2] and are extended in the current article. The revised model requires modification of the PDE material balance on primary radicals generated by water radiolysis:

\[
\frac{\partial [(PR')]}{\partial t} = \frac{\Gamma(x) R_{PR} \phi V_R}{\phi} - \frac{r_{(PR)}}{\phi} \frac{[(PR')] \partial \phi}{\partial t}
\]

where [(PR')] is the concentration of primary radicals, \(\Gamma(x)\) identifies zones receiving or not receiving radiation, \(R_{PR}\) is the rate of generation of primary radicals (dose rate times G factor), \(\phi\) is the volume fraction occupied by the aqueous phase, \(V_R\) is the total volume of the phantom and \(r_{(PR)}\) is the rate of consumption of primary radicals by subsequent reactions. Fuxman et al. [1,2] used their model to study edge enhancement at a sharp interface between irradiated and un-irradiated zones. They used \(\Gamma(x)\) to distinguish locations that receive radiation (\(\Gamma(x) = 1\)) from locations that do not (\(\Gamma(x) = 1\)). When investigating the effects of PDD in the current work, \(\Gamma(x)\) provides depth-dose information in the form of cubic splines. All other PDEs remain the same as those of Fuxman et al. [1,2], and boundary conditions were revised to permit heat loss through the front and back walls of the phantom shown in Fig. 2. Updated values of model parameters [5] that were fitted using experimental data [6,7], are used in the revised model.

2.3. Model Solution

Cubic polynomial equations were fitted using the spline toolbox in Matlab\textsuperscript{TM}. The complete system of 29 PDEs was solved using the VLUGR2 solver within Fortran [8]. Note that the PDE model can also be solved using the pdepe subroutine in Matlab\textsuperscript{TM}, but simulation times are prohibitively long. The PDEs were solved to predict the mass of polymer and the temperature vs. depth at different times. Additional simulations were performed to examine the importance of monomer diffusion and temperature effects. Simulations with diffusion turned off (\(D_{M1} = 0\)) were compared with simulations...
that account for diffusion \( (D_{M1} = 4.1 \times 10^{-6} \text{ cm}^2/\text{min}) \), and simulations with heat effects turned off \((T = 20^\circ \text{C everywhere})\) were compared with simulations that account for the heat released by polymerization. All simulations considered the total given dose at \( d_{max} \) to be 5 Gy; for the Co\(^{60} \) \( \gamma \)-radiation simulations, a dose rate was set to 2 Gy/min, for all other radiation beams the dose rate was 4 Gy/min.

![Figure 2](image)

Figure 2. Schematic diagram of the irradiation of a simulated phantom with a PDD curve, where \( d_{max} \) represents the location of maximum absorbed dose, and \( d_b \) is the depth of the back wall. A value of \( d_b = 10 \text{ cm} \) was used for all simulations, except for the 20 MeV electron beam, which used \( d_b = 15 \text{ cm} \) because of deeper penetration.

3. Results and Discussion

Simulation results showing the amount of polymer formed 24 hours post irradiation are shown in Fig. 3b along with the corresponding depth-dose data in Fig. 3a. The amount of polymer formed for each type of radiation has a shape similar to its depth-dose curve. There are, however, some noticeable differences between the shapes of the curves, especially near the position of maximum dose. For example, the polymer formation curve for the Co\(^{60} \) \( \gamma \)-radiation has a more pronounced maximum than does its PDD curve. An examination of the cause of this difference is provided below.

![Figure 3](image)

Figure 3. Comparison between (a) the depth-dose curves and (b) the amount of polymer formed 24 post irradiation for Co\(^{60} \) \( \gamma \)-radiation, 6 MV X-ray photon beam and 9 MeV electron beam.

3.1. Diffusion Effects

Selected simulation results comparing the model predictions with and without diffusion effects are presented in Fig. 4. Table 1 shows the percent difference in the mass of polymer formed at the location of maximum dose, with and without diffusion. Note that, when diffusion is turned on, the location of maximum dose \( (d_{max}) \) does not correspond perfectly to the location of maximum polymer formation, with this peak shifted slightly towards the adjacent area receiving less radiation where
monomers are more plentiful. The simulations show that diffusion effects are more prominent near the depth of maximum dose than at greater depths where dose gradients are small and diffusion effects can hardly be noticed (see Fig. 4a). For high MV photon beams and high MeV electron beams, where the PDD curves are smoother than for Co\textsuperscript{60} \(\gamma\)-radiation, diffusion effects have only a minor influence on the amount of polymer formed (see Fig. 4b and Table 1).

![Figure 4. Comparison between normal simulations and simulations without diffusion for: a) Co\textsuperscript{60} \(\gamma\)-radiation and 6 MeV electron beam, b) 12 and 16 MeV electron beams, 24 hours post irradiation.](image)

Table 1. Amount of polymer formed 24 hours post irradiation at the location of maximum absorbed dose for simulations with and without diffusion and with and without temperature effects.

| Radiation type          | Polymer formed (g/L) | Percent increase with D | Percent increase with T |
|-------------------------|----------------------|-------------------------|-------------------------|
|                         | with D and T         | without D               | without T               |
| Co\textsuperscript{60} \(\gamma\)-radiation | 39.72     | 38.24                   | 39.21                   | 3.87       | 1.30        |
| 6 MV X-ray photon beam  | 37.57     | 37.33                   | 37.05                   | 0.64       | 1.40        |
| 15 MV X-ray photon beam | 37.5      | 37.38                   | 36.64                   | 0.32       | 2.34        |
| 6 MeV electron beam     | 38.12     | 37.11                   | 37.35                   | 2.72       | 2.06        |
| 9 MeV electron beam     | 37.47     | 36.96                   | 37.19                   | 1.38       | 0.75        |
| 12 MeV electron beam    | 37.39     | 37.21                   | 37.01                   | 0.48       | 1.03        |
| 16 MeV electron beam    | 37.24     | 37.21                   | 36.78                   | 0.08       | 1.25        |
| 20 MeV electron beam    | 37.34     | 37.31                   | 36.27                   | 0.08       | 2.95        |

3.2. Temperature Effects

The temperature of the system increases as polymerization occurs, and then eventually decreases due to heat loss through the walls of the phantom. Regions where higher amounts of radiation are delivered achieve higher temperatures. Since temperature increases the rate of polymerization, more polymer tends to form in highly irradiated areas, than if the system were isothermal [7]. Simulation results showing temperature profiles and comparing the model with and without temperature effects are presented in Fig. 5b and Table 1. Note that the temperature is higher for the 20 MeV electron beam than for other types of radiation because the high dose region was more extensive (given the broad shoulder in the depth-dose curve). This results in more of the phantom volume being irradiated to a higher dose and more polymer forms. As expected, the total amount of polymer formed decreases when the temperature effects are removed from the model. Larger differences between predictions with and without temperature effects occur near the maximum dose depth than deeper in the phantoms where polymerization and heat generation rates are lower. In all simulated cases, the amount of additional polymer formed at \(d_{max}\) is less than 2.5%, except for 20 MeV which had an increase of nearly 3%, due to the higher temperature, which is shown in Fig. 5a.
4. Conclusions and Recommendations
A fundamental PDE model was developed to simulate depth-dose effects in PAG dosimeters. Both diffusion and temperature effects influence the amount of polymer formed at various locations. Diffusion effects are more apparent for Co$^{60} \gamma$-radiation (a 3.9% increase in polymer formed at the location of maximum dose) than for other types of radiation with flatter maxima. Temperature effects are larger when more radiation is delivered. These simulation results indicate that when calibration curves are developed using depth-dose information, more accurate results may be obtained by avoiding the depth of maximum dose, particularly for Co$^{60} \gamma$-radiation.

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