Supplementary information

Section 1. *Supplementary tables*

Table S1. Composition of simulated tissues/materials

Structure	Composition (mass fraction)
Cylinder (polyoxymethylene)*	0.400 C, 0.067 H, 0.533 O
Female soft tissue**	0.106 H, 0.315 C, 0.024 N, 0.547 O, 0.001 Na, 0.002 P, 0.002 S, 0.001 Cl, 0.002 K
Bladder (full)**	0.108 H, 0.035 C, 0.015 N, 0.830 O, 0.003 Na, 0.001 P, 0.001 S, 0.005 Cl, 0.002 K
Intestine**	0.106 H, 0.115 C, 0.022 N, 0.751 O, 0.001 Na, 0.001 P, 0.001 S, 0.002 Cl, 0.001 K
Cortical bone**	0.034 H, 0.155 C, 0.042 N, 0.435 O, 0.001 Na, 0.103 P, 0.003 S, 0.225 Ca, 0.002 Mg
Air***	0.0123 C, 75.0325 N, 23.6007 O, 1.2743 Ar

** Röchling/Piedmont Plastics, Technical data sheet – Sustarin (R) H (acetal homopolymer Delrin). Web (last accessed December 2022): https://www.piedmont-plastics.com/products/acetal; ** D.R. White, R.V. Griffith, and I.J. Wilson, ICRU Report 46, Photon, Electron, Proton and Neutron Interaction Data for Body Tissues (International Commission on Radiation Units and Measurements, 1992); *** M.J. Rivard, B.M. Coursey, L.A. DeWerd et al., Update of AAPM Task Group No. 43 Report: A revised AAPM protocol for brachytherapy dose calculations, Med Phys 2004; 31: 633-674*

Table S2. Relative dose differences (EQD_2 EBRT + BT) of target and OAR volumes across all 61 patients

DVH metric		Average ±STD dose difference (%)		
		MC vs. TG43	MC_{water} vs. TG43	MC vs. MC_{water}
$Vagina_{5mm}$ (Gy_3)	$D_{0.1cc}$	–43.9 ±14.8	–43.1 ±14.9	–1.4 ±0.8
	$D_{0.5cc}$	–15.8 ±7.4	–14.9 ±7.4	–1.2 ±0.4
	D_{1cc}	–8.8 ±4.6	–7.8 ±4.6	–1.1 ±0.4
	D_{2cc}	–5.6 ±3.0	–4.6 ±2.9	–1.1 ±0.5
	D_{4cc}	–4.1 ±2.0	–3.0 ±1.9	–1.1 ±0.4
$Vagina_{5mm\text{-}CTV}$ (Gy_3)	$D_{0.1cc}$	–21.5 ±20.4	–20.4 ±20.6	–1.3 ±0.7
	$D_{0.5cc}$	–7.2 ±9.1	–6.1 ±9.2	–1.2 ±0.3
	D_{1cc}	–4.4 ±5.8	–3.2 ±5.8	–1.2 ±0.3
	D_{2cc}	–2.7 ±3.5	–1.5 ±3.5	–1.2 ±0.3
	D_{4cc}	–1.9 ±2.2	–0.8 ±2.1	–1.1 ±0.3
CTV (Gy_{10})	D_{50}	–2.4 ±0.7	–1.5 ±0.7	–0.9 ±0.2
	D_{90}	–2.0 ±0.6	–1.2 ±0.6	–0.8 ±0.2
	D_{98}	–2.2 ±0.7	–1.4 ±0.7	–0.8 ±0.2
GTV (Gy_{10})	D_{90}	–2.3 ±0.9	–1.5 ±0.9	–0.8 ±0.2
	D_{98}	–2.3 ±0.7	–1.5 ±0.7	–0.8 ±0.2
IR-CTV (Gy_{10})	D_{90}	–1.3 ±0.5	–0.7 ±0.4	–0.6 ±0.2
	D_{98}	–1.3 ±0.7	–0.8 ±0.6	–0.5 ±0.2
Bladder (Gy_3)	$D_{0.1cc}$	–1.0 ±1.1	–0.5 ±1.1	–0.5 ±0.2
	D_{2cc}	–1.0 ±0.7	–0.6 ±0.7	–0.5 ±0.2
Rectum (Gy_3)	$D_{0.1cc}$	–1.1 ±0.6	–0.2 ±0.5	–0.9 ±0.3
	D_{2cc}	–1.1 ±0.4	–0.3 ±0.3	–0.7 ±0.3
Sigmoid (Gy_3)	$D_{0.1cc}$	–0.1 ±1.7	0.4 ±1.8	–0.5 ±0.3
	D_{2cc}	–0.5 ±0.7	–0.1 ±0.6	–0.4 ±0.3

Table S3. Absolute dose differences (EQD_2 EBRT + BT) of target and OAR volumes across all 61 patients

DVH metric		Average ±STD dose difference ($Gy_{\alpha/\beta}$)		
		MC vs. TG43	MC_{water} vs. TG43	MC vs. MC_{water}
$Vagina_{5mm}$ (Gy_3)	$D_{0.1cc}$	–1,016.3 ±910.3	–1,002.1 ±906.5	–14.2 ±9.9
	$D_{0.5cc}$	–101.4 ±93.3	–96.0 ±91.7	–5.4 ±2.7
	D_{1cc}	–37.5 ±33.3	–33.6 ±32.0	–3.9 ±2.1
	D_{2cc}	–16.8 ±13.2	–13.8 ±12.2	–3.0 ±1.7
	D_{4cc}	–8.7 ±5.9	–6.4 ±5.2	–2.3 ±1.2
$Vagina_{5mm\text{-}CTV}$ (Gy_3)	$D_{0.1cc}$	–206.9 ±327.8	–201.6 ±324.5	–5.3 ±5.7
	$D_{0.5cc}$	–23.7 ±36.1	–21.1 ±35.2	–2.5 ±1.6
	D_{1cc}	–10.1 ±14.9	–8.1 ±14.1	–2.0 ±1.2
	D_{2cc}	–4.6 ±6.4	–3.0 ±5.9	–1.6 ±0.8
	D_{4cc}	–2.4 ±3.1	–1.2 ±2.6	–1.2 ±0.6
CTV (Gy_{10})	D_{50}	–3.0 ±1.1	–1.9 ±1.0	–1.1 ±0.3
	D_{90}	–1.8 ±0.6	–1.1 ±0.6	–0.7 ±0.2
	D_{98}	–1.8 ±0.6	–1.2 ±0.6	–0.6 ±0.2
GTV (Gy_{10})	D_{90}	–2.4 ±1.1	–1.5 ±0.8	–0.9 ±0.3
	D_{98}	–2.1 ±0.7	–1.3 ±0.6	–0.7 ±0.2
IR–CTV (Gy_{10})	D_{90}	–0.9 ±0.4	–0.5 ±0.4	–0.4 ±0.1
	D_{98}	–0.8 ±0.6	–0.5 ±0.5	–0.3 ±0.1
Bladder (Gy_3)	$D_{0.1cc}$	–1.1 ±1.2	–0.6 ±1.3	–0.5 ±0.3
	D_{2cc}	–0.9 ±0.7	–0.5 ±0.6	–0.4 ±0.2
Rectum (Gy_3)	$D_{0.1cc}$	–0.9 ±0.6	–0.2 ±0.5	–0.7 ±0.4
	D_{2cc}	–0.7 ±0.3	–0.2 ±0.2	–0.5 ±0.2
Sigmoid (Gy_3)	$D_{0.1cc}$	–1.0 ±7.9	–0.5 ±7.6	–0.5 ±0.5
	D_{2cc}	–0.4 ±0.5	–0.1 ±0.5	–0.3 ±0.2

Section 2. ***Dose profiles: Monte Carlo versus treatment planning system***

In this section, we provide dose profiles to further detail the TG43 conditions dose differences observed between the treatment planning system (TPS) and MC in this work. First, dose profiles will be shown for a single ^{192}Ir flexi–source source in water with full backscatter conditions for MC. Both calculations have identical dose grids of 1 × 1 × 1 mm^3. For MC, 1 × 10^7 histories were run. Figure S1 shows axial 1D profiles directly through the source dwell position in both the TPS and MC. The profiles are generally in agreement within 3% outside 3 mm. At 3 mm and closer, the agreement worsens. Of note, 3 mm is the limit for most TG43 parameter data tables, and at 3 mm and closer, the TPS must extrapolate beyond provided data to calculate dose. The central voxel contains the source, where dose deposited in the source itself is not scored in MC. The MC dose in the central voxel is non–zero due to a volume averaging effect since the source diameter is approximately 0.85 mm, which is smaller than the bounds of the 1 × 1 × 1 mm^3 voxel. In contrast, the TPS uses extrapolation for dose calculation up to a maximum dose value; in this case, 8× is the prescription dose that was arbitrarily set to 5 Gy.

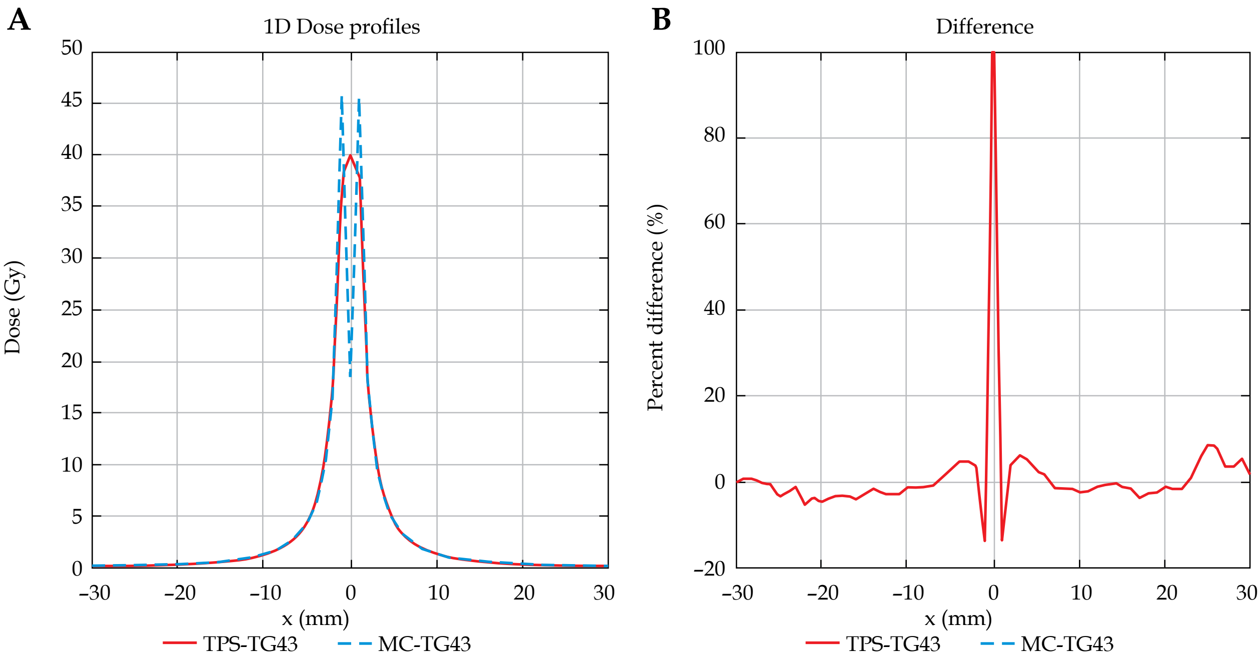

Fig. S1. A) 1D dose profiles axially through a single ^{192}Ir flexi–source in water as calculated in the TPS and in MC. **B**) Percent difference between MC with respect to the TPS

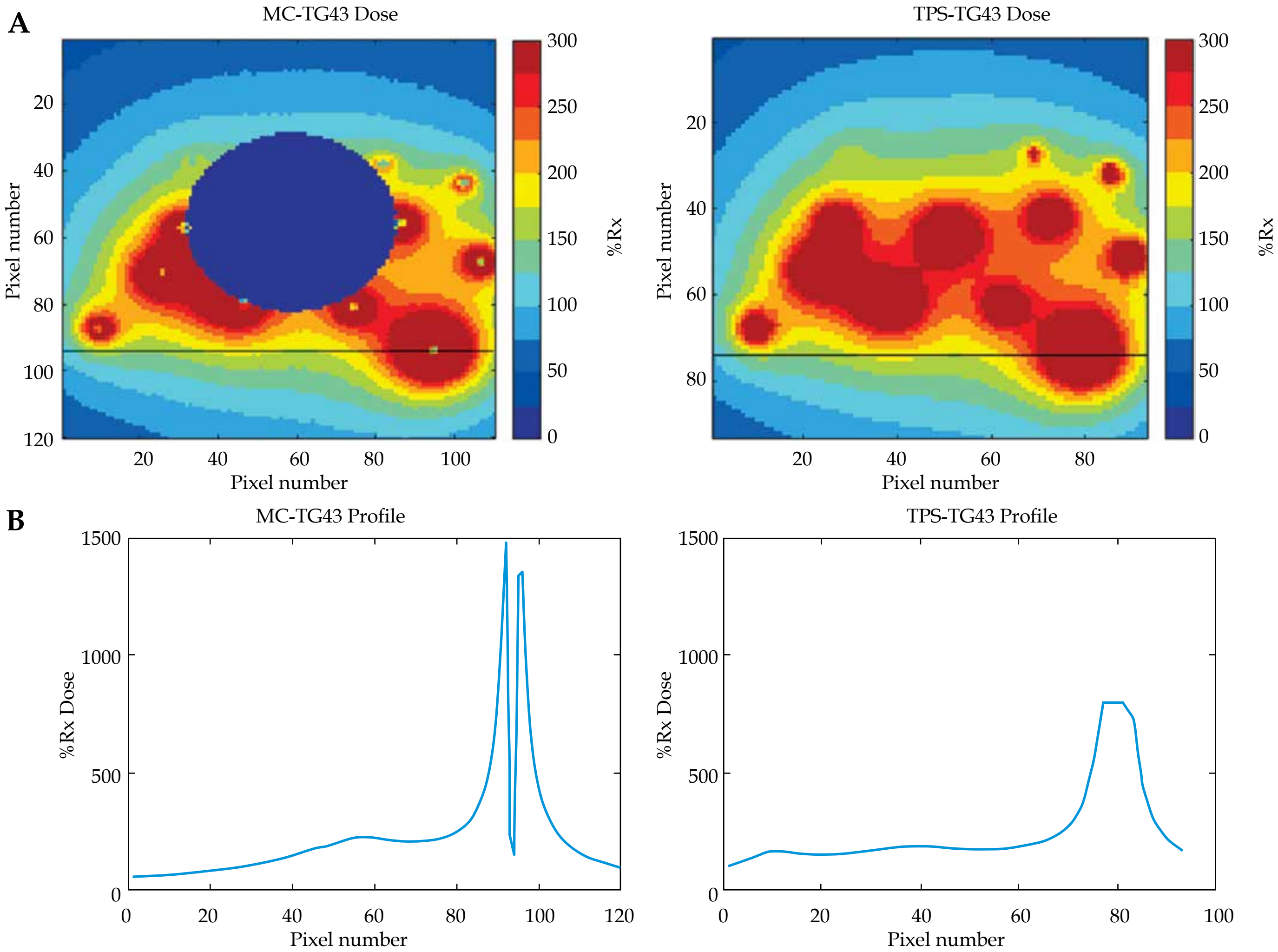

Fig. S2. The axial dose distribution of a patient with the worst agreement between the TPS and MC (the same distributions are shown in Figure 2), then shows 1D profiles going directly through a source dwell position. Note that the dose was calculated with different dose grids as TPS used 1 × 1 × 1 mm^3 voxels while MC used the patient voxels of 0.3 × 0.3 × 1.5 mm^3, so the profiles shown are closely matched but do not have the same width and location in the TPS and MC. However, the profiles in Figure S2 show the effects of calculation differences between the TPS and MC in a clinical scenario. MC dose is calculated without any maximum dose setting but is not scored inside sources, while TPS dose is calculated up to a threshold maximum dose. Therefore, evaluating very small vaginal dose DVH values on the order of individual source volumes will result in large discrepancies between the TPS and MC, especially when many dwell positions occur inside the vaginal contour. **A**) MC (water) and TPS axial dose distributions for a patient with the largest vaginal DVH discrepancies between calculation methods. **B**) 1D dose profiles corresponding to the black line are shown in dose distributions