BEAM DYNAMICS TRACKING SIMULATIONS FOR UK XFEL UNDER THE INFLUENCE OF LONG-RANGE DIPOLE WAKEFIELDS

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Abstract

The baseline design for the proposed UK XFEL (United Kingdom X-ray Free Electron Laser) facility includes main linear accelerating linacs, which are comprised of 600 L-band 9-cell TESLA style superconducting (SC) RF cavities, which will accelerate a 1-MHz repetition-rate irregularly spaced composite electron beam comprised of varying bunch charges up to an energies of 8 GeV. Here the TESLA cavities are simulated and the dipole modes excited by the beam are characterised in order to calculate the long-range transverse wakefields (LRTWs). We track the particles through 1 km under the influence of these LRTWs using the PLACET code and evaluate the transverse emittance dilution of the electron beam.

INTRODUCTION

Coherent X-ray free-electron lasers (XFELs) enable probing of atomic-scale structure and femtosecond dynamics across applications such as biomolecular processes, chemical reactions, and extreme states of matter. Efficient lasing requires control of the electron beam energy spread (σ_γ) and emittance (ϵ_n). For the UK XFEL, the target fractional energy spread is $\sigma_\gamma \leq 10^{-2}\%$ to maintain resonance. Large emittance reduces beam–radiation coupling and degrades performance. Here, we investigate the unmitigated emittance growth ($\Delta\epsilon/\epsilon_0$) through the UK XFEL lattice. For a 600 pC bunch with a baseline $\epsilon_\mathrm{n} = 0.7$ mm mrad, and considering $\epsilon_\mathrm{n} = 0.46$ mm mrad with no LRTWs applied, $\Delta\epsilon/\epsilon_0$ should remain below 50%.

The UK XFEL main linac comprises three accelerating sections separated by two magnetic chicanes [1]. It contains 600 L-band (1.3 GHz) 9-cell TESLA-type cavities: 16, 152, and 432 in sections 1–3, respectively, arranged in cryomodules of eight cavities. Sixteen third-harmonic cavities precede BC1, followed by eight compensating L-band cavities. This study considers unmitigated transverse kicks only (see Fig. 1 and Table 1).

SIMULATIONS AND BENCHMARKING

CST Simulations

Higher order modes (HOMs) in the beamline vacuum contribute to emittance dilution via long-range transverse wakefields (LRTWs), requiring beam dynamics simulations for assessment. Here we use PLACET [2] to evaluate transverse wakes produced through bunch-driven excitation of dipole modes, with bunches radially offset by σ of their transverse Gaussian distribution. PLACET requires the frequency, quality and kick factors of each HOM, delivered by CST [3] simulations.

Table 1: Linac Cavity Configuration

	Cavity Name	**Pop.**	**Freq. [GHz]**	**Gradient [MV/m]**	**Phase [deg]**
Section 1	LIN1	16	1.3	17.686	58.0
	HARM	16	3.9	3.094	-90.0
Section 2	COMP	8	1.3	6.827	65.0
	LIN2	152	1.3	13.593	61.1
Section 3	LIN3	432	1.3	13.657	90.0

An axially symmetric model of a TESLA 9-cell L-band cavity was built in CST and benchmarked against established results [4]. The loss factor for each mode was calculated at a fixed radial offset by first integrating $E_z(r,\theta,z)$ along that offset trajectory to derive the accelerating voltage (V_acc)

$$V_\mathrm{acc}(r) = \int_{-L/2}^{L/2} E_z(r,\theta,z)\exp\left(\frac{-i\omega_n z}{c}\right)dz, \tag{1}$$

where L is the longitudinal length of the structure. The longitudinal loss parameter of a mode is the energy lost by a charged particle traversing a cavity per unit charge squared and is given by

$$k_\parallel = \frac{|V_\mathrm{acc}|^2}{4U}, \tag{2}$$

where c is the speed of light in a vacuum, ω_n is the angular frequency of the n^th mode, and U is the stored energy.

From the offset longitudinal loss factor, the kick factor of the mode can be calculated using

$$K = \frac{k_\parallel c}{\omega_0 L r^2}, \tag{3}$$

where r is the radial coordinate of the longitudinal line integral and L is the length or period of the cell or cavity. See Fig. 2 for a Brillouin diagram comparison between [4] (using MAFIA) and this study's CST results and Fig. 3 for a kick factor comparison, where significant kicks agree within 1%. In both Figs. 2 and 3, WMM and WEE represent Wanzenbergs results with an electric-electric and magnetic-magnetic boundary respectively, while WMON refers to results from [4] for the first passband of the monopole modes.

Particle Tracking Simulations

The effects of LRTWs caused by resonant modes stimulated by transiting electron bunches are calculated by

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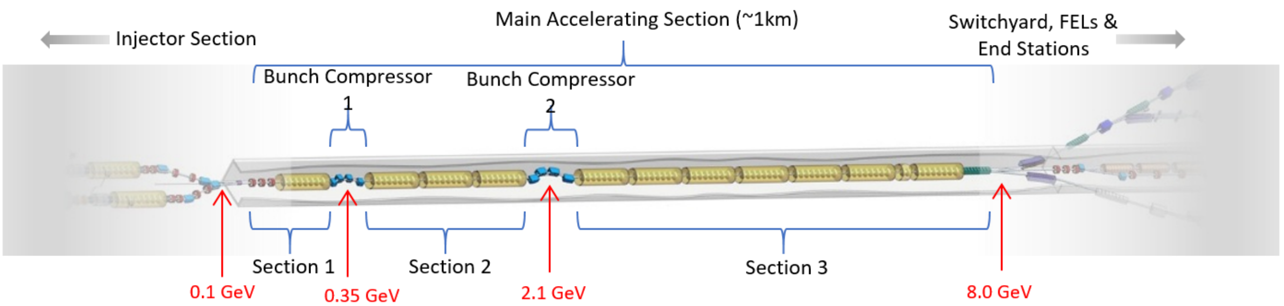

Figure 1: The main accelerating section of the proposed UK XFEL facility [1].

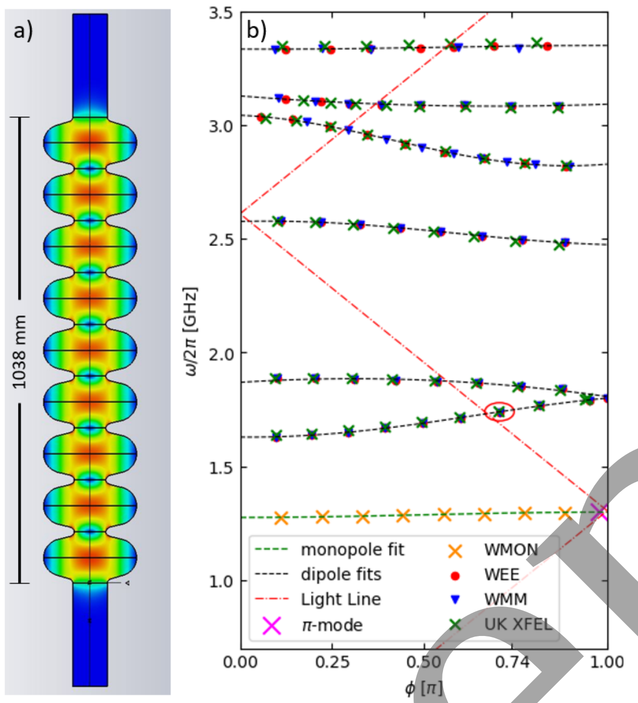

Figure 2: Benchmarking the CST model against known results [4] for the L-band TESLA cavity. a) The TM_{010} π-mode E-field distribution. b) The Brillouin diagram for the first monopole and first 6 dipole pass-bands. Results from [4] are depicted in the legend with the prefix ’W’.

PLACET [2] which was benchmarked against an existing ELEGANT [5] model of the main accelerating section, see Fig. 4 for a comparison between the horizontal phase space at the end of the lattice in ELEGANT and PLACET.

As electron bunches propagate through the lattice, wakes (W) in each TESLA cavity build up until reaching a steady state where contributions from initial bunches have rung out, controlled by the Q_0 value of each contributing mode, as shown in Eq. 4 from [6]

$$W(s) = 2\,\mathrm{Im}\left\{\sum_{n=1}^{N} K_n e^{i\omega_n s/c} e^{-\omega_n s/2Q_n c}\right\} U(s), \qquad (4)$$

where K_n is the kick factor of the n^{th} mode, s is the longitudinal coordinate, Q_n is the quality factor of the n^{th} mode, and here $U(s)$ is the unit step function, defined as 1 if $s > 0$ and 0 if $s < 0$.

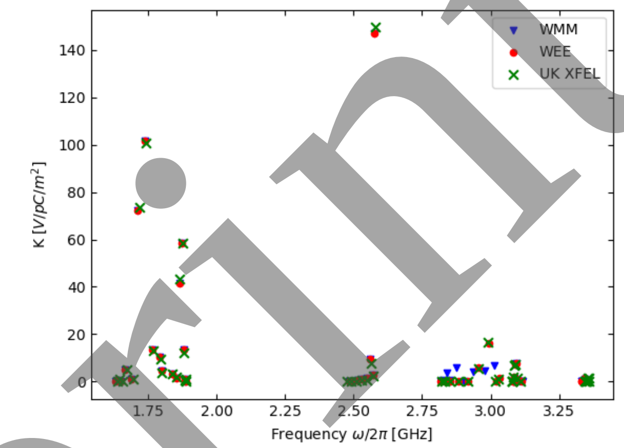

Figure 3: Frequency vs. Kick factor plot for the dipole modes, comparing derived results (UKXFEL) to trusted, published numbers by Wanzenberg [4]. Here, the kick factors > 20 V/pC/m^2 will dominate.

The steady state can be represented by the summed wake (S) derived by adding together the contributions from all bunches until they have rung out to below a level that contributes significantly (Eq. 5)

$$S = \sum_{i=1}^{N} W(s_i). \qquad (5)$$

The LRTWs for each TESLA cavity were activated in the PLACET lattice and their effect on the normalised horizontal emittance (ϵ) was gauged with regard to a 600 pC bunch after a composite beam comprised of 75 pC bunches at a bunch repetition rate of 250 kHz and 150 pC bunches at 500 kHz. See Fig. 5 for a visualisation of the time/charge structure of the composite beam.

Due to the intensive computational requirements of these multi-bunch simulations the Q_0 of the fundamental accelerating TM_{010} π-mode was set at 10^6 and all other values of Q_0 scaled accordingly.

RESULTS

The results of the PLACET simulations of the composite beam’s effect on a trailing 600 pC bunch is shown in Fig. 6. The horizontal normalised emittance is diluted by 73.5%.

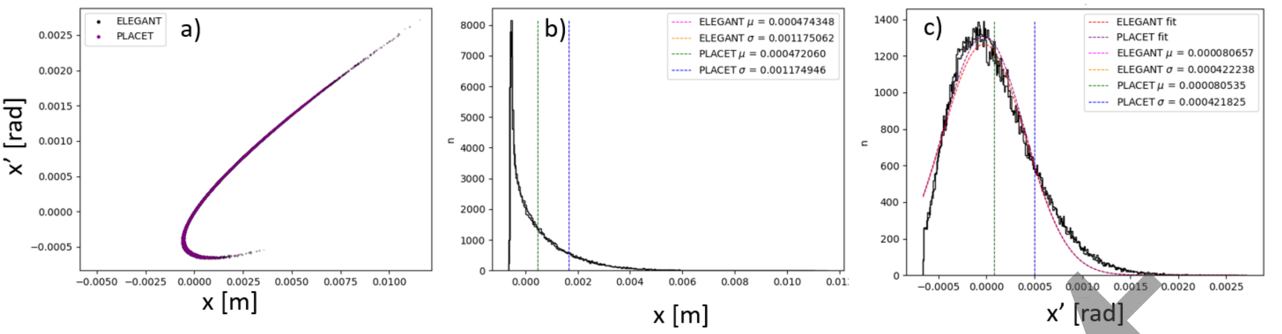

Figure 4: Benchmarking PLACET (purple data) against ELEGANT (black data). a) The horizontal phase space of a 75 pC bunch at the end of the main accelerating section. b) and c) are histograms of the horizontal position angles respectively. There is good agreement between the results delivered by tl

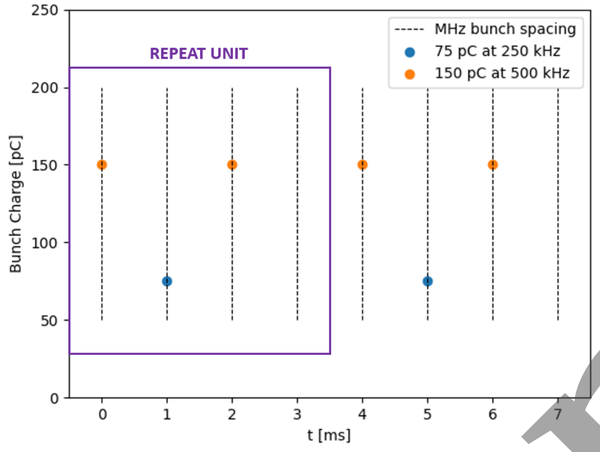

Figure 5: Illustration of the composite beam time/charge structure. Each repeat unit contains three bunches, with a trailing 600 pC bunch embedded within the 1 MHz rhythm. Its horizontal normalised emittance is tracked and reported in Fig. 6.

Emittance dilution is defined as

$$\frac{\Delta\epsilon}{\epsilon_0} = \frac{|\epsilon_\perp - \epsilon_0|}{\epsilon_0} \times 100\% \,. \tag{6}$$

A function was fitted to the data relating the number of bunches in the simulation to emittance dilution

$$\frac{\Delta\epsilon}{\epsilon_0} = A(1 - e^{-\Gamma n}), \tag{7}$$

where A is the steady-state value of $\Delta\epsilon/\epsilon_0$, Γ is a damping coefficient and n is the number of bunches in the simulated composite beam. Here, $A = 73.49\%$ and $\Gamma = 2.2 \times 10^{-4}$, the fit has an R^2 value of 0.9954.

DISCUSSION

The unmitigated normalised horizontal emittance dilution of UK XFEL's composite beam is 73.5%. Next steps are to confirm PLACET LRTW results with RF-Track [7] or ELEGANT [5], then simulate long-range *longitudinal* wakes

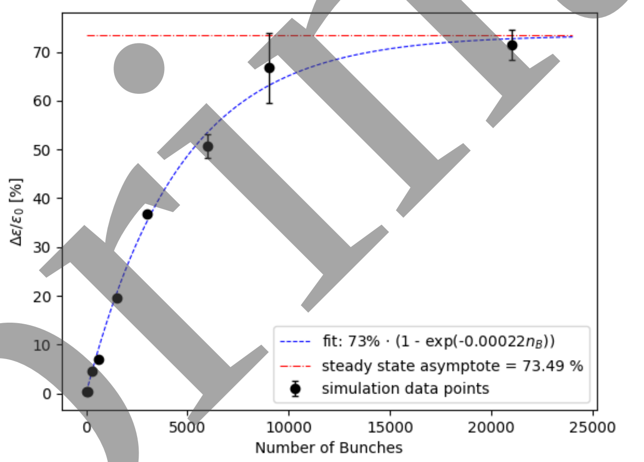

Figure 6: PLACET [2] results for the effect of the LRTW on ϵ_n as a function of the number of bunches in a simulation. The error bars display the standard deviation in $\Delta\epsilon/\epsilon_0$ judged at the final ten lattice elements.

(LRLWs) and assess their effect on energy spread. Finally, LRTWs and LRLWs for the third-harmonic cavities should be quantified, since wakes from these smaller structures may be more substantial.

ACKNOWLEDGEMENTS

The authors thank Nirav Joshi, Aaron Farricker, Daniel Schulte, Andrea Latina and Paula Desiré.

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