

Balance of bunch compression and emittance preservation for high-brightness x-ray free electron laser injectors

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This paper presents two conceptual low-energy injector configurations optimized for high-brightness, high-repetition-rate XFELs. The designs were evaluated at a nominal bunch charge of 150 pC using multiobjective optimization techniques and further assessed through start-to-end simulations incorporating collective effects to determine their suitability for delivering high-brightness beams under FEL-relevant conditions. One of the injector design configurations employs a hybrid rf and magnetic compression scheme, while the second relies solely on two-stage rf compression. Start-to-end simulations through the main linac, including collective effects, were performed to assess the suitability of each design for meeting XFEL requirements. The results highlight the critical role of longitudinal charge distribution symmetry in maintaining beam quality during acceleration and compression, and demonstrate that appropriately balancing compressibility, emittance preservation, and phase space linearity is essential for meeting the stringent demands of XFEL operation.

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I. INTRODUCTION

In recent decades, x-ray free electron laser (XFEL) facilities—driven by advanced linear accelerators capable of producing high-brightness, ultrarelativistic electron bunches—have revolutionized x-ray generation by delivering coherent, laserlike pulses on the femtosecond scale with unprecedented brightness, enabling entirely new classes of experiments in ultrafast science and structural imaging [1,2]. The first lasing was achieved in 2005 at the Deutsches Elektronen-Synchrotron (DESY) [3] in the vacuum ultraviolet range, with capabilities later extended into the soft x-ray regime. A major milestone was reached in 2009 when the Linac Coherent Light Source (LCLS) at

the SLAC National Accelerator Laboratory produced the first hard x-ray lasing, marking the beginning of a new era in x-ray science [4]. Since then, continuous efforts have been made to push the boundaries of XFEL performance, including the development of advanced concepts such as multicolor and two-pulse x-rays, variable polarization states, and high spectral purity, along with achieving increased brightness, subfemtosecond and attosecond pulse durations, and high-repetition rates [5].

The performance and efficiency of an XFEL are ultimately determined by the quality of the electron bunch as well as the undulator properties; therefore, it is essential to underline the importance of the six-dimensional (6D) brightness of the bunch as a key figure of merit:

$$B_{6D} = \frac{Q}{\epsilon_{n,x}\epsilon_{n,y}\epsilon_{n,z}} \approx \frac{I/\sigma_E}{\epsilon_{n,x}\epsilon_{n,y}}, \quad (1)$$

where Q is the bunch charge, I is the bunch peak current, σ_E is the uncorrelated energy spread, and $\epsilon_{n,x}$, $\epsilon_{n,y}$, and $\epsilon_{n,z}$ are the normalized horizontal, vertical, and longitudinal emittances. Equation (1) indicates that a high-brightness electron bunch comprises a combination of low transverse emittance

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and energy spread with a high peak current. The relationship between the final 6D brightness of the bunch before lasing, undulator parameters, and the photon wavelength can be expressed as

$$B_{6D, \text{final}} \approx \frac{I}{\lambda \sigma_E} \frac{32\pi^2}{c \lambda_u (1 + a_w^2)}, \quad (2)$$

where λ is the radiation wavelength, λ_u is the undulator period length, c is the speed of light, and a_w is the undulator parameter [6]. This relation demonstrates that high 6D brightness is essential for achieving high gain and efficient energy extraction in the FEL process. However, high-brightness beam characteristics alone are not sufficient, as the bunch repetition rate also directly determines the scientific capabilities of an XFEL facility [7–9]. Therefore, a high-repetition-rate XFEL injector must deliver electron bunches with high 6D brightness that can be preserved through the main linac to enable efficient FEL lasing, ensuring the beam quality that meets the demanding specifications for coherent x-ray generation across diverse scientific applications.

Achieving high-repetition rates is a significant engineering challenge, primarily due to radio-frequency (rf) power dissipation on the cavity walls [10]. Consequently, continuous wave (cw) operation with high frequency and high peak field is not feasible using conventional designs. cw operation of normal-conducting (NC) gun-based injectors can be implemented by reducing the gun field to approximately 30 MV/m and operating at a frequency typically below 250 MHz. Meanwhile, superconducting rf (SRF) gun technology is a promising alternative for applications requiring higher rf fields and frequencies for cw operation.

Two continuous wave XFEL facilities are progressing toward full operation: LCLS-II at SLAC in the U.S., which has achieved first lasing but is not yet running at its design repetition rate [11], and SHINE in China, which remains under construction but has successfully commissioned its very high frequency (VHF) gun. Both facilities feature similar injector beamline designs: an NC VHF gun is followed by a two-cell 1.3 GHz NC buncher cavity for bunch compression, and a booster section for acceleration composed of 1.3 GHz TESLA-type SRF cavities [12]. The design of an NC cw VHF gun operating at 187 MHz was first demonstrated at LBNL for the Advanced Photoinjector Experiment (APEX) [13]. The APEX gun was designed to operate at 750 kV with a cathode field of 20 MV/m and an average rf power of 90 kW. LCLS-II uses a VHF gun design similar to the APEX gun, operating at 185.7 MHz. Although the gun was designed for a voltage gain of 750 kV, it typically runs at 650 kV, corresponding to a photocathode gun field of 17.5 MV/m [14]. It is worth noting that the LCLS-II high-energy low-emittance injector upgrade has initiated R&D studies to develop an SRF VHF gun as an independent injector in parallel with the existing NC VHF gun, aiming to reduce emittance and enable future

photon energy upgrades for an extended photon science program [15,16]. Building on the LCLS-II developments, a VHF gun operating at 216.67 MHz was designed for the SHINE injector, with a voltage of 878 kV, a cathode field of 30 MV/m, and an average rf power of 95.8 kW [17].

The European XFEL has also been investigating the feasibility of cw operation through its high-duty-cycle upgrade program since 2014. The European XFEL currently employs a pulsed normal-conducting rf gun to generate high-repetition-rate bunch trains, which are then accelerated in 1.3 GHz TESLA-type SRF cavities without any dedicated bunch compression within the injector beamline, unlike the LCLS-II and SHINE injectors. A planned upgrade to a 1.3 GHz L-band SRF gun is under development; its design specifies an on-axis peak electric field of 40 MV/m, and early prototypes have demonstrated fields up to 60 MV/m [18].

In this paper, two alternative low-energy injector beamline configurations for the UK XFEL are presented. A conceptual VHF gun design is introduced and its performance is evaluated under varying laser pulse durations to investigate the trade-off between longer bunches for emittance preservation and the need for subsequent compression. The requirement for longitudinal bunch compression is then established, and two injector layouts are described and discussed in detail. In design-I, bunch compression is achieved through a hybrid scheme combining rf and magnetic techniques. A 650.0 MHz single-cell linearizer placed immediately after the gun corrects rf curvature, followed by initial compression in a 216.67 MHz prebuncher and acceleration in five-cell 650.0 MHz SRF cavities. Final linearization is applied using nine-cell 1.3 GHz TESLA-type cavities before the beam enters a symmetric C-shaped magnetic chicane. In design-II, a purely rf-based, two-stage velocity bunching scheme is employed, beginning with a 216.67 MHz normal-conducting prebuncher and continuing in a five-cell 650.0 MHz SRF buncher, followed by acceleration in nine-cell 1.3 GHz TESLA-type SRF cavities. Both designs are optimized to deliver bunch durations below 20 ps, with their respective priorities discussed in the corresponding sections of this paper. One should note that the bunch duration here refers to the full temporal length of the bunch, rather than an rms or FWHM value. Both configurations are subsequently tracked through the main linac to assess their impact on beam quality at 8 GeV. The paper is structured as follows. Section II describes the VHF gun design and beam-dynamics framework. Section III details the optimization and beamline studies for design-I and design-II. Section IV presents the start-to-end tracking results through the main linac. Section V discusses potential challenges across all beamline elements—including and beyond the injector and main linac optics employed—and Sec. VI concludes with the outcomes of the comparative study and its implications for XFEL performance.

II. VHF GUN DESIGN

A frequency of 216.67 MHz was selected for the VHF gun, corresponding to the 6th subharmonic of the planned 1.3 GHz main linac frequency for the UK XFEL. This choice, rather than the 7th subharmonic option, was made to maximize gun performance by enabling a higher achievable surface electric field. Two VHF gun designs were developed and optimized, following the methodology described in Ref. [19]. The first design—referred to as the traditional geometry—follows the conventional re-entrant layout, similar to previous VHF gun designs [13,17], aiming to maintain proven performance characteristics. In this configuration, the extrusion at the front of the gun, measured from the end of the accelerating gap, is limited to 2 cm. The second design—referred to as the relaxed geometry—removes this constraint, allowing a larger extrusion at the front. This sacrifices some compactness but increases the achievable rf voltage at the same input power limit, enabling higher bunch energy at the gun exit to mitigate space charge effects further. One should note that the relaxed geometry approach is similar to the single-cell configuration considered during the APEX2 gun development [19], before a final two-cell design was eventually selected.

For both designs, the re-entrant VHF gun geometry was parameterized in SUPERFISH [20] using 19 variables, which served as inputs for a multiobjective genetic optimization implemented through the PySuperfish framework [21]. The NSGA-II algorithm [22], within the DEAP library [23], was employed to explore the parameter space, with the objectives of maximizing the rf voltage and minimizing the required rf input power, while maintaining a fixed cathode field of 30 MV/m. The optimization was subject to constraints on the rf frequency (216.67 ± 3 MHz), maximum surface electric field (37 MV/m), and peak power density (35 W/cm^2). The resulting Pareto fronts for the traditional and relaxed geometries are shown in Fig. 1(a), with the corresponding optimized gun geometries illustrated in Figs. 1(b) and 1(c), respectively. The axial electric field profiles for both designs are presented in Fig. 1(d).

An input power of 90 kW was selected [highlighted in Fig. 1(a)], based on current VHF gun technologies [13,17] and constrained by the available high-power rf transport capabilities. In future work, this limit will be reassessed to determine whether higher power operation is feasible, for example, by increasing the number of cavity input couplers. An rf voltage of 826 kV is achieved in the traditional design, compared to 1102 kV in the relaxed geometry. Further investigation will be required to assess potential limits related to the size and positioning of the gun solenoids for the relaxed design. Moreover, neither gun design has yet been evaluated for susceptibility to multipactor effects, and mitigation strategies may reduce the achievable performance if multipactor becomes significant. Nevertheless, due to its higher applicable accelerating voltage, improved slice emittance, and bunch energy at

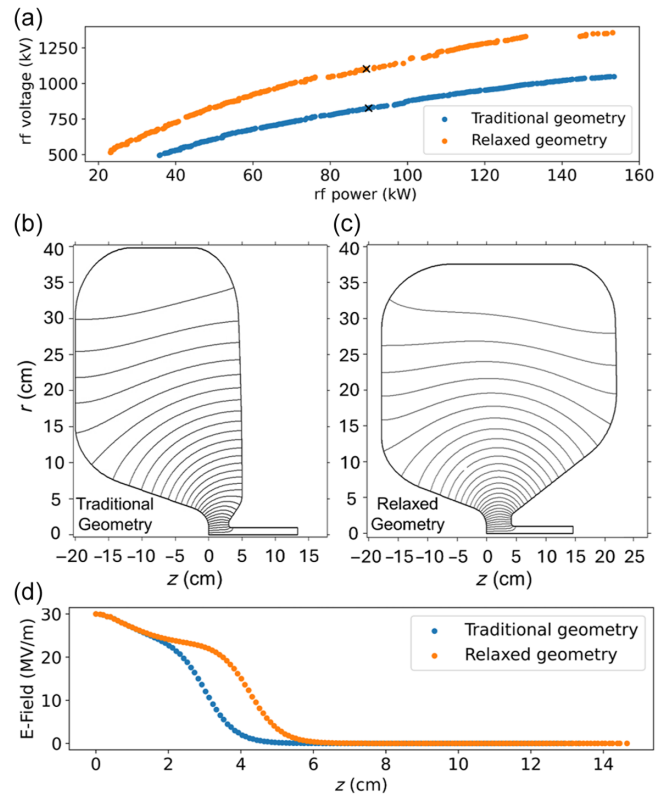


FIG. 1. (a) Pareto fronts for each gun design. The selected design is marked with a black cross. (b) Optimized traditional gun geometry. (c) Optimized relaxed gun geometry. (d) Peak on-axis electric field for each gun design.

the gun exit, the relaxed geometry was selected for further injector design studies presented in this work.

The performance of the relaxed gun geometry was evaluated in terms of the minimum achievable slice emittance using OPAL simulations, with space charge effects enabled [24]. Simulations were performed for a 150 pC bunch using 100,000 macroparticles and a 3D rectangular mesh of 32 grid points per dimension. The slice emittance is determined by multiple sources, including intrinsic cathode emittance, emission current density, linear and nonlinear space charge forces, rf aperture limitations, and aberrations induced by the gun solenoid. These contributions can be balanced by optimizing the laser spot size and pulse duration to minimize the overall transverse slice emittance.

Figure 2 shows the dependence of the slice emittance—defined as the average emittance of the three central slices out of nine equally spaced longitudinal slices along the bunch—on the laser parameters for the relaxed gun geometry. These central slices were used to assess gun performance due to their relevance to the FEL process, where the highest current density and best transverse coherence are typically achieved.

A Cs_2Te photocathode with a thermal emittance of 0.85 mm mrad/mm rms was used to generate the electron bunch, with a flat-top laser profile applied both transversely

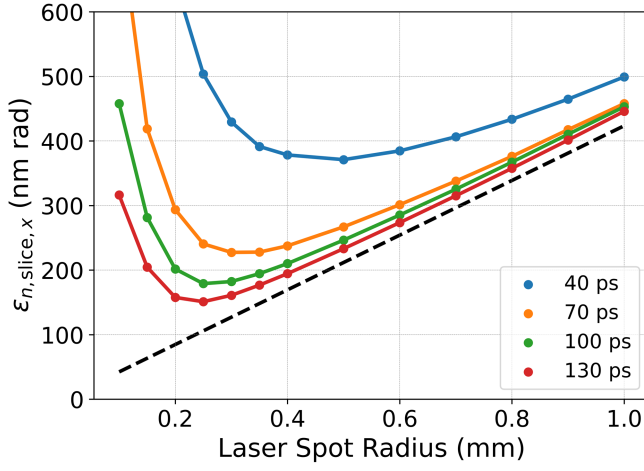


FIG. 2. Average slice emittance of the three central slices of the bunch at the emittance compensation point, shown as a function of laser spot size and pulse duration for the relaxed gun geometry.

and longitudinally in all simulations. For reference, the theoretical cathode-limited slice emittance was also calculated using the method described in Ref. [25] and is shown with dashed lines for comparison. Increasing the laser pulse duration reduces the slice emittance, as the lower emission current density results in weaker space charge forces. The smallest simulated slice emittance is achieved with the longest laser pulse duration of 130 ps, corresponding to 10° of the gun frequency. Decreasing the laser spot size reduces the slice emittance by minimizing the cathode contribution while enabling the use of smaller transverse laser profiles. However, reducing the spot radius below 0.25 mm leads to emittance blowup during emission due to excessive current density. The simulation results indicate that achieving low slice emittance at the gun favors the use of long laser pulses.

III. INJECTOR BEAMLINE DESIGN OPTIONS

In this section, alternative injector beamline designs are introduced and discussed, collectively referred to as the low-energy injector section, where the bunch energy typically remains below 200 MeV. The injector beamline is defined as the portion of the accelerator upstream of the main linac. The optimized beamline layouts are presented,

followed by a detailed discussion of the optimization procedures and the resulting transverse and longitudinal properties of the compressed bunch in each case. All beam dynamics analysis for the low-energy injector design studies, including both individual and multiobjective optimization runs [26], were carried out using OPAL simulations with space charge effects enabled. A 3D rectangular mesh with 32 grid points per spatial dimension and 100,000 macroparticles was employed, representing a bunch charge of 150 pC. Field calculations were conducted using OPAL's fast Fourier transform-based particle-mesh solver, chosen for its numerical stability and accuracy in modeling collective interactions.

A. Injector design-I

Design-I beamline is developed to maximize the 6D brightness of the electron beam. To achieve this, the design process is guided by minimizing the three primary beam quality objectives: the transverse core emittance (see Appendix C 1), the skewness of the longitudinal charge distribution (see Appendix C 2), and the bunch duration. The aim is to carefully balance the bunch compression and emittance preservation while shaping the charge density along the bunch.

The beamline optimization process is structured in two stages: the first stage involves initial rf bunch compression (see Appendix B 1) and acceleration, while the second focuses on further acceleration, linearization, and final magnetic compression (see Appendix B 2). Figure 3 shows the layout used for the initial multiobjective optimization, based on the variables listed in Table I, which targets the characterization and optimization of early-stage bunch compression.

Three separate optimization studies were performed, each employing a single-cell prebuncher cavity at one of three frequencies—216.67, 650.0, or 1300.0 MHz. Identical cavity geometries were maintained across all cases to enable a direct performance comparison. A linearizer cavity, operating at the third harmonic of the VHF gun frequency, was placed immediately downstream of the gun to compensate for the second- and fourth-order rf nonlinearities introduced during emission—particularly relevant since the gun operates near on crest. The linearizer also improves the

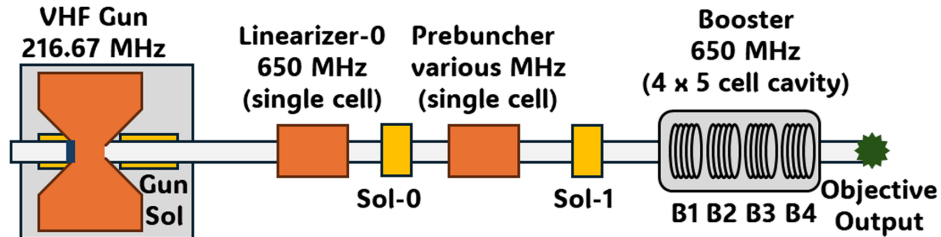


FIG. 3. First stage of the optimization for design-I, where the electron bunch is generated, the longitudinal phase space is linearized, and initial rf compression and acceleration are performed.

TABLE I. Optimization variables for the first stage of the design-I beamline used in multiobjective simulations, as shown in Fig. 3.

Parameter	Range	Unit
Laser spot radius	[0.15 1.5]	mm
Laser duration	[40 130]	ps
Gun phase	[−15 15]	°
Gun sol strength	[30 100]	mT
Linearizer-0 field	[0.5 7.5]	MV/m
Linearizer-0 phase	[−190 − 170]	°
Sol-0 strength	[30 100]	mT
Prebuncher field	[0.5 7.5]	MV/m
Prebuncher phase	[−120 − 60]	°
Sol-1 strength	[50 250]	mT
Booster (B1–B4) field	[10 20]	MV/m
Booster (B1 and B2) phase	[−15 15]	°
Booster (B3 and B4) phase	On crest	°

performance of the initial bunch compression by correcting for the second-order longitudinal dispersion (T_{566}) in the subsequent drift section. Finally, a booster cryomodule consisting of four five-cell SRF cavities operating at 650 MHz was included to accelerate the compressed bunch, facilitating a comparative study of the compression limits and the lowest achievable transverse core emittance for the three prebuncher configurations. Figure 4 shows the Pareto fronts for transverse core emittance and bunch duration across the considered configurations.

The skewness of the longitudinal charge distribution, used as the third optimization objective, is represented by a color bar with a common scale applied to all Pareto fronts. Among the Pareto front results obtained from different configurations, the 216.67 MHz prebuncher provides the best compromise between minimal transverse core emittance and reduced skewness of the longitudinal charge distribution for a compressed bunch duration of approximately 40 ps, as shown in Fig. 4(a). The enhanced

compression performance achieved with the 216.67 MHz prebuncher is attributed to the longer initial bunch generated at the gun, enabled by the lower-frequency cavity. The longer bunch helps mitigate space charge-induced emittance growth during the early stages of transport. Based on these results, the combination of the 650 MHz linearizer and the 216.67 MHz prebuncher was selected for the initial bunch compression stage in the remainder of this study. The parameters obtained from the simulation, given with their ID in Fig. 4, were adopted as the optimal configuration for evaluating bunch compression performance and beam dynamics.

Figure 5 shows the bunch energy and higher-order energy spread profiles at the entrance of the booster.

The bunch energy profile is symmetric, with a peak current of 6.3 A and a longitudinal charge distribution skewness of 0.011. The majority of the charge is concentrated in the center of the bunch (between −10 and 10 ps), where the energy-bunch duration correlation is almost linear, while the head and tail regions exhibit curvature with relatively small amounts of charge as shown in Fig. 5(a). The higher-order energy spread profile is also symmetric, with most of the charge located around zero deviation as shown in Fig. 5(b). The rms higher-order energy spread is 8.1 keV. One should note that the calculation of higher-order energy spread is performed by applying a fourth-order polynomial fit to the energy profile and subtracting the contributions up to second order to isolate the higher-order components. A fourth-order fit is used to ensure an accurate match with the energy-bunch duration correlation and to avoid underestimating the higher-order energy spread, as can occur in some approaches developed for beam dynamics analysis [27], which can result in a reduction of the high-order energy spread by up to a factor of 2.

The second stage of the optimization was performed using the beam parameters obtained from the first optimization, covering further acceleration, linearization, and the final magnetic compression of the bunch. This two-stage approach

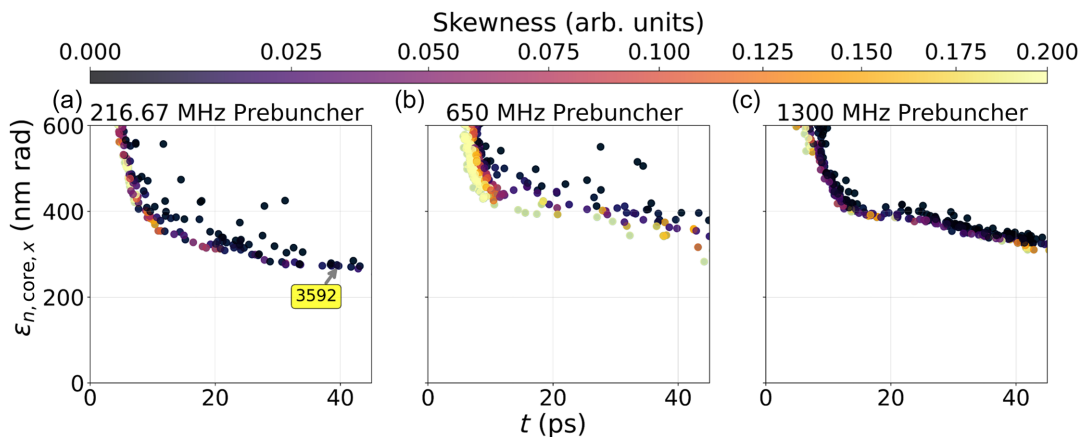


FIG. 4. Pareto front obtained from the multiobjective optimization for different buncher cavities used in design-I beamline shown in Fig. 3.

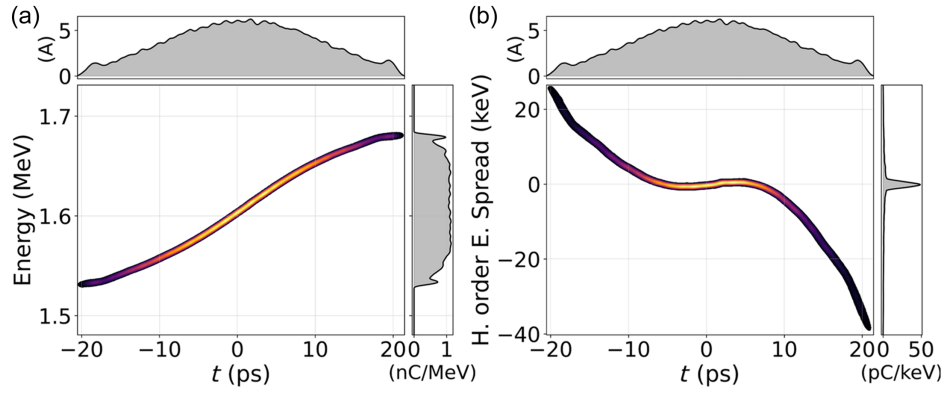


FIG. 5. (a) Bunch energy and (b) higher-order energy spread at the booster entrance, with the charge density indicated by the color scale from brighter (higher charge density) to darker (lower charge density). The 1D profiles along the top and side of each plot show the corresponding charge distributions.

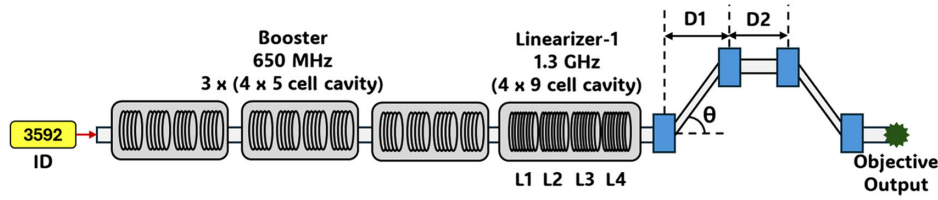


FIG. 6. Second stage of the optimization for design-I, where the electron bunch is further accelerated by three additional booster cryomodules (in addition to the one used in the first stage), the longitudinal phase space is linearized, a linear energy chirp is imparted, and final magnetic compression is performed.

was adopted to reduce significantly the computational cost, as performing a full start-to-end optimization in a single stage would be prohibitively time consuming. Additionally, the second stage has no impact on the upstream beam dynamics, justifying the use of preoptimized parameters as input. This strategy ensures consistency while maintaining computational efficiency. Figure 6 shows the layout used for the second stage, and the additional optimization variables are listed in Table II.

The three additional booster cryomodules operating at 650 MHz were used on crest to accelerate the bunch to

around 187 MeV, maintaining the beam quality achieved after the first cryomodule. A dedicated linearizer cryomodule consisting of four nine-cell 1.3 GHz TESLA-type cavities was operated off crest to provide the necessary energy chirp and to compensate for the second- and fourth-order rf-induced nonlinearities introduced by the booster cryomodules, after which the bunch energy drops to 140 MeV. Figure 7 shows the Pareto front obtained for radial core emittance, final bunch duration, and skewness at the end of the magnetic chicane (see Appendix B2). One should note that the bunch was confirmed to be in the emittance-dominated regime prior to entering the magnetic chicane (see Appendix C3).

The radial core emittance, calculated as the geometric mean of the horizontal and vertical emittances, is used as a single objective in the multiobjective optimization. It shows a small change of less than 10% down to a bunch duration of 15 ps, while the skewness of the longitudinal charge distribution increases with the compression factor. Therefore, a change in skewness of up to 0.1 was considered tolerable. Based on this criterion, the optimized parameters associated with the simulation ID shown in the Pareto front were selected as the optimal solution.

Figure 8 shows the bunch energy and higher-order energy spread profiles before and after the chicane.

The linearizer is operated using a combination of near on-crest and off-crest phases. The near on-crest setting

TABLE II. Optimization variables for the second stage of the design-I beamline used in multiobjective simulations, as shown in Fig. 6. The angle θ represents the exit angle of the first and third dipoles and the entrance angle of the second and fourth. The drift between the first and second dipoles (and likewise between the third and fourth) is denoted D1, while D2 denotes the drift space between the second and third dipoles.

Parameter	Range	Unit
Linearizer-1 field (L1–L4)	[5 30]	MV/m
Linearizer-1 phase	[−200 − 135]	°
θ	[5.0 35.0]	°
D1	[0.25 3.0]	m
D2	[0.25 3.0]	m

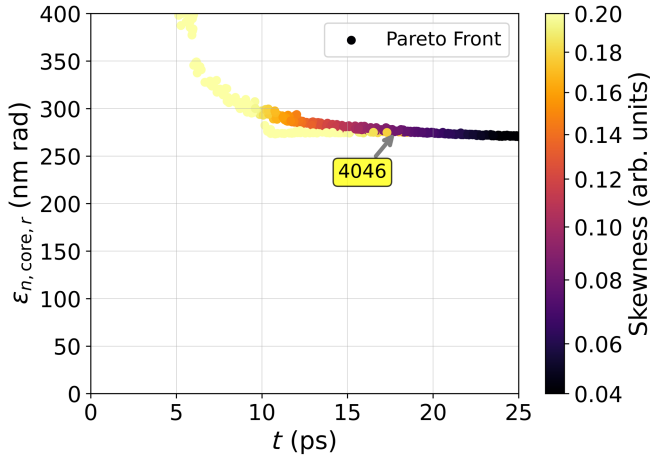


FIG. 7. Pareto front obtained from the multiobjective optimization of the final magnetic compression stage.

reduces curvature at the head and tail of the bunch, while the off-crest operation—where the sinusoidal rf field locally approximates a linear slope—provides the required chirp for the chicane and helps to preserve the rms higher-order energy spread, as shown in Figs. 8(a) and 8(b), respectively. The resulting linear energy chirp of -3.35 m^{-1} corresponds to an R_{56} value of 15 cm for a compression factor of 2, as calculated using Eq. (B3). After

linearization, the bunch centroid shifts to -0.66 ps , with a slightly reduced skewness of 0.011 and a bunch duration of 37.2 ps at the entrance of the chicane. The energy—bunch duration correlation is preserved during compression in the chicane, while the rms higher-order energy spread increases to 15.3 keV as shown in Figs. 8(c) and 8(d), respectively. The mean relative energy spread is found to be 2×10^{-4} , and the final bunch duration of 16.9 ps is achieved with a skewness of 0.08.

The evolution of the normalized rms projected, horizontal, and vertical core emittances, as well as the bunch duration along the beamline, is shown in Fig. 9.

Initially 86.5 ps at the gun exit, the bunch duration is compressed to 16.9 ps, corresponding to a compression factor of 5.1. At the compensation point downstream of the gun, the normalized projected and core emittances in the horizontal and vertical planes were 372.1 and 257 nm rad, respectively. Transverse axisymmetry is preserved up to the chicane entrance, where the normalized projected and core emittances are 312.6 and 267 nm rad, respectively. However, due to the dipole focusing in a single plane inherent to the magnetic chicane, transverse axisymmetry is no longer preserved, leading to an increase in the horizontal core emittance to 285 nm rad. In contrast, the vertical core emittance remains almost unchanged at 268 nm rad; this minor increase can be attributed to numerical noise.

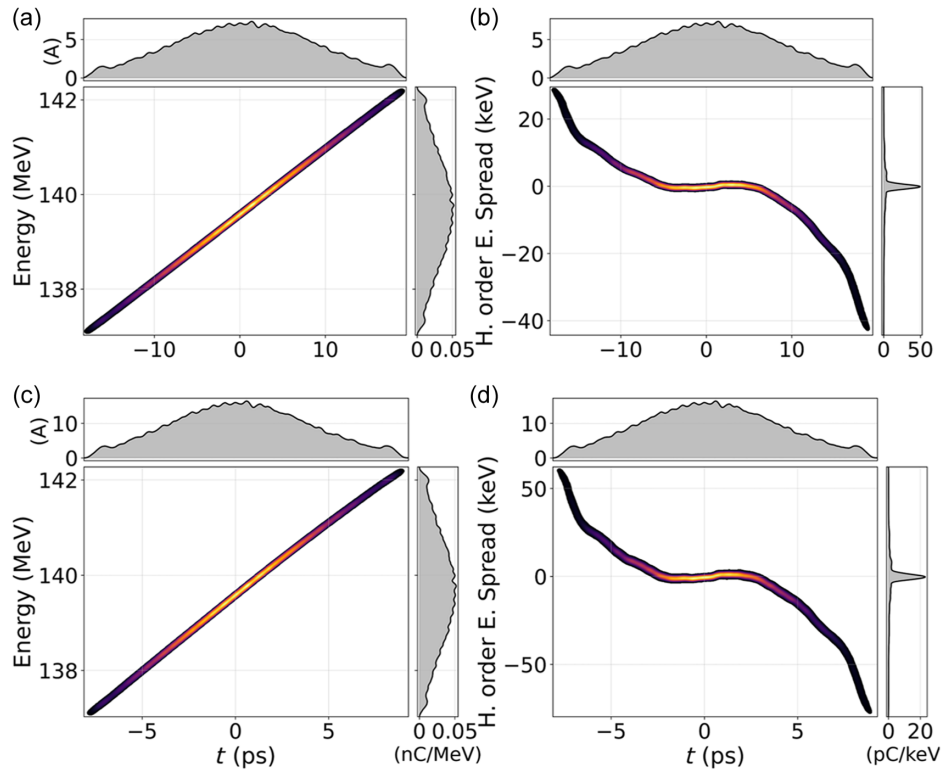


FIG. 8. Bunch energy and higher-order energy spread profiles before (a), (b) and after the chicane (c), (d) above and below, respectively. The color scale indicates the charge density, and 1D projections of the charge distribution are displayed on the top and side of each figure.

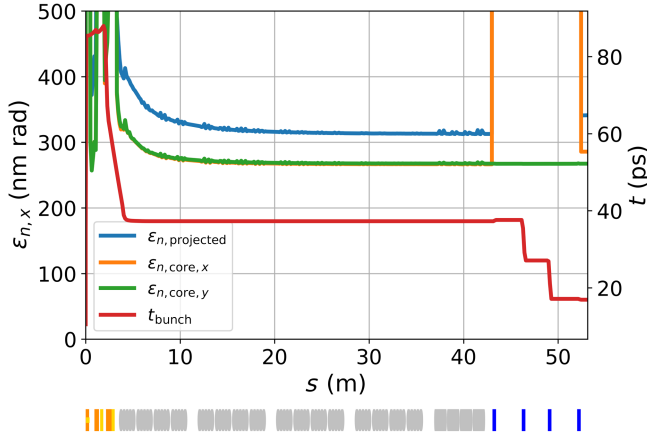


FIG. 9. Evolution of the normalized projected emittance, horizontal and vertical core emittances, and bunch duration along the design-I beamline.

Figure 10 shows the horizontal and vertical phase spaces before and after magnetic compression.

Prior to the chicane, both slice alignment and core emittance are well preserved in the horizontal and vertical phase spaces as shown in Figs. 10(a) and 10(b). However, following the chicane, slice alignment degrades in the horizontal plane, resulting in increased core emittance caused by the chicane optics and space charge effects. The emittance increase is more pronounced at the bunch extremities, where phase-space shifts are greater. Although the core emittance definition effectively excludes these shifts from the analysis, an 18 nm rad increase still occurs

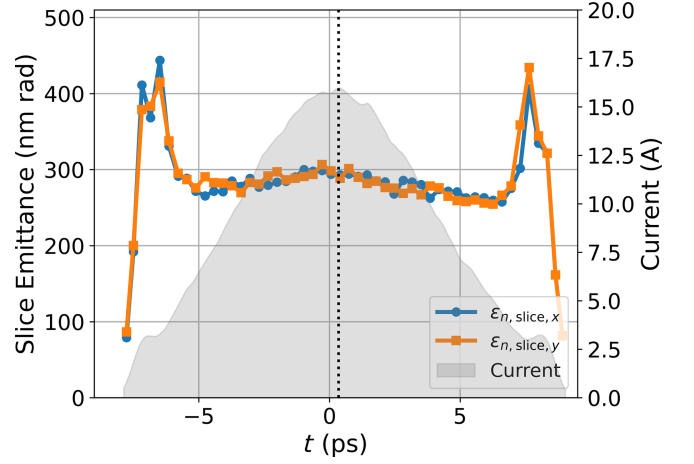


FIG. 11. Horizontal and vertical slice emittances along the bunch, shown together with the final 1D current profile. The bunch is divided into 50 slices to resolve variations in emittance along the bunch.

within the core as demonstrated in Fig. 10(c). In the vertical plane, the slice alignment remains almost unchanged, as the dispersive effects do not directly influence vertical motion. Although the bunch diverges as illustrated in Fig. 10(d), which is indicated by the phase space orientation, downstream after the chicane, the vertical core emittance experiences only a negligible growth.

Figure 11 shows the horizontal and vertical slice emittances along the bunch, along with the final 1D current profile.

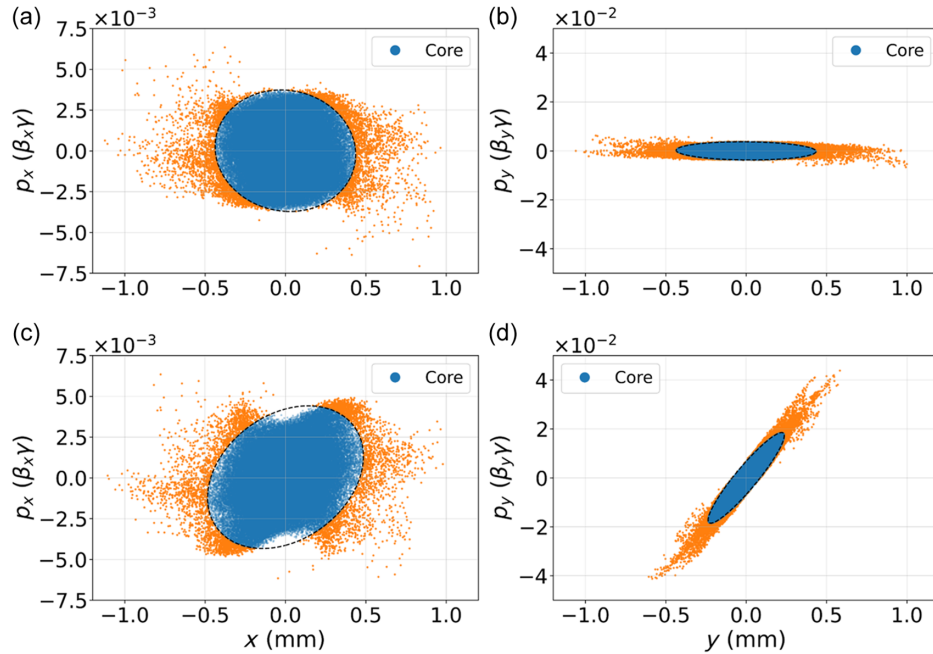


FIG. 10. Horizontal (a), (c) and vertical (b), (d) phase spaces before and after magnetic compression (above and below, respectively). The scales are kept identical within the horizontal and vertical phase spaces to enable a meaningful comparison. Particles shown in blue correspond to those within the core emittance ellipse.

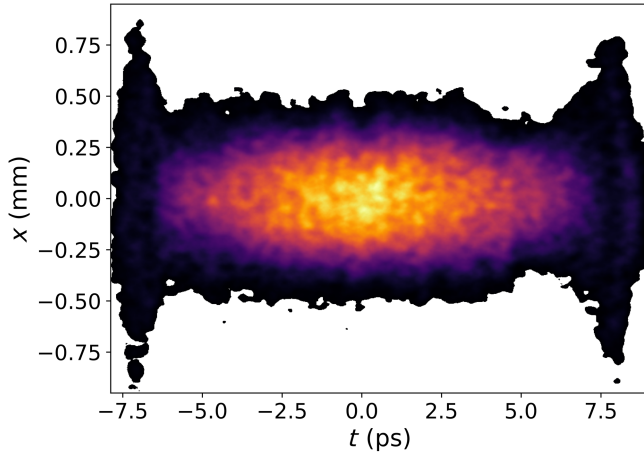


FIG. 12. Beam projection in the horizontal-longitudinal plane. The bunch exhibits a symmetric profile with the peak current density concentrated at its center.

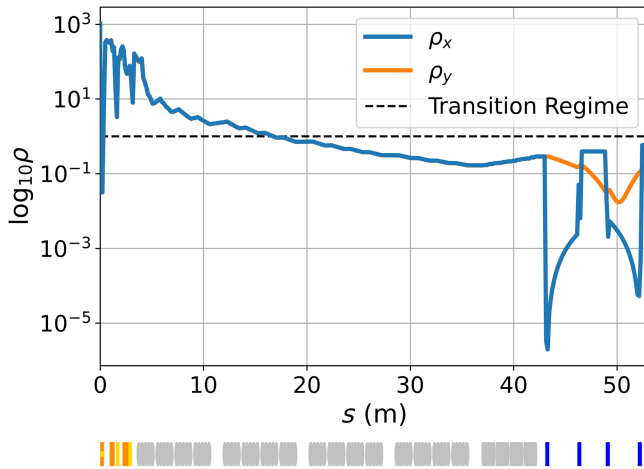


FIG. 13. Evolution of the laminarity parameter along the design-I beamline. The positions of beamline elements are indicated below the plot.

The head and tail slice emittances are approximately 1.5 times higher than those of the center slices, an inevitable consequence of the sinusoidal rf field in which off-crest particles experience nonlinear voltage curvature (higher-order energy chirp) and phase-dependent transverse focusing. However, the majority of the charge is symmetrically

concentrated in the center of the bunch, which has a peak current of 16 A. To provide a more detailed view of the charge distribution, the current density profile of the beam projection in the horizontal-longitudinal plane is illustrated in Fig. 12.

The beam projection clearly illustrates a symmetric, high-current density central region, where the majority of the bunch charge is concentrated, consistent with the optimized low-skewness longitudinal profile. Additionally, the head and tail exhibit broader horizontal spread, indicative of the high slice emittance at the bunch extremities. Nevertheless, the current density in these outer regions is significantly lower than that at the center of the bunch. Overall, the final current density along the bunch confirms the efficacy of the optimization approach in maintaining a well defined, symmetric charge distribution.

Figure 13 shows the evolution of the laminarity parameter (see Appendix C3) along the beamline, confirming that the optimized bunch remains in the emittance-dominated regime at the end of the injector beamline.

The bunch is significantly influenced by space charge forces before acceleration. As acceleration begins, these effects gradually diminish, and by the second cryomodule—where the beam energy reaches approximately 80 MeV—the bunch enters the emittance-dominated regime. Continued acceleration further reduces the transverse laminarity parameter, effectively rendering space charge forces negligible. However, the laminarity increases in the second linearizer due to a temporary reduction in beam energy and an increase in beam size, even though the emittance remains constant. Within the chicane, variations in beam size and emittance cause it to fluctuate between the dipoles, affecting the horizontal and vertical planes differently. Nevertheless, the final values of the laminarity parameter in both the horizontal and vertical directions remain below unity, confirming that the bunch is emittance dominated and ready for injection into the main linac.

B. Injector design-II

Design-II adopts a two-stage rf compression scheme, in contrast to the hybrid compression approach employed in design-I. In this configuration, the skewness of the longitudinal charge distribution is not included as an optimization objective, since the physics of two-stage rf compression leads

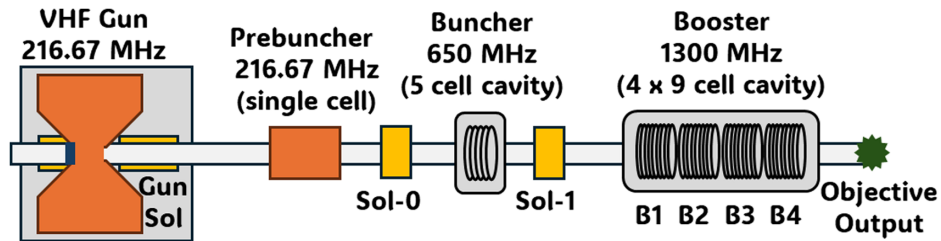


FIG. 14. Two-stage rf compression layout for design-II.

TABLE III. Variables used in multiobjective simulations to optimize the design-II beamline layout shown in Fig. 14.

Variable	Range	Unit
Laser spot radius	[0.15 1.5]	mm
Laser duration	[40 130]	ps
Gun phase	[−15 15]	°
Gun sol strength	[30 100]	mT
Prebuncher field	[0.5 7.5]	MV/m
Prebuncher phase	[−120 − 60]	°
Sol-0 strength	[30 100]	mT
Buncher field	[0.5 7.5]	MV/m
Buncher phase	[−80 − 10]	°
Sol-1 strength	[50 250]	mT
Booster (B1–B4) field	[10 30]	MV/m
Booster (B1 and B2) phase	[−15 15]	°
Booster (B3 and B4) phase	On crest	°

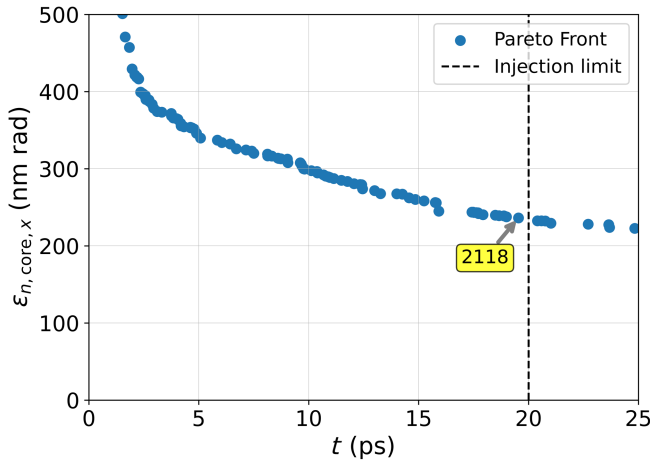


FIG. 15. Pareto front obtained from the multiobjective optimization simulations based on the design-II layout shown in Fig. 14.

to a naturally skewed charge profile and a curved longitudinal phase space. This behavior arises primarily from the second buncher operating far off crest, where velocity bunching is effectively applied. Therefore, the optimization strategy accepts longitudinal asymmetry in favor of achieving a lower core emittance at the end of the injector.

Figure 14 shows the beamline layout used in the multiobjective optimization for design-II, with the corresponding variables listed in Table III.

A single-cell 216.67 MHz NC prebuncher located after the VHF gun, followed by a five-cell 650 MHz SRF buncher cavity (Appendix A2), enables two-stage rf bunch compression in design-II. To preserve the bunch energy before the first compression stage, the use of a linearizer cavity after the gun was intentionally excluded from the optimization. The multiobjective optimization focused on minimizing the transverse core emittance and bunch length as two primary objectives. This approach prioritizes beam quality in the high-current region of the bunch, while tolerating extended tails resulting from nonlinear compression effects.

The Pareto front obtained from the multiobjective optimization is shown in Fig. 15.

Considering the bunch duration limit required for injection into the booster, Pareto front data with bunch durations exceeding 20 ps were excluded. Therefore, the simulation highlighted in Fig. 15 was selected as the optimal solution and used for further analysis. The laser spot radius and duration used in this simulation were 0.36 mm and 107.5 ps, respectively. Both the prebuncher and buncher cavity phases were selected in the accelerating phase by the optimizer.

Figure 16 shows the bunch energy and higher-order energy spread profiles at the entrance of the booster.

The nonlinear rf contributions, originating from the gun and accumulating through the prebuncher and buncher cavities, result in a curved longitudinal phase space at the booster entrance due to successive compression stages occurring at nonzero-crossing phases, which also lead to

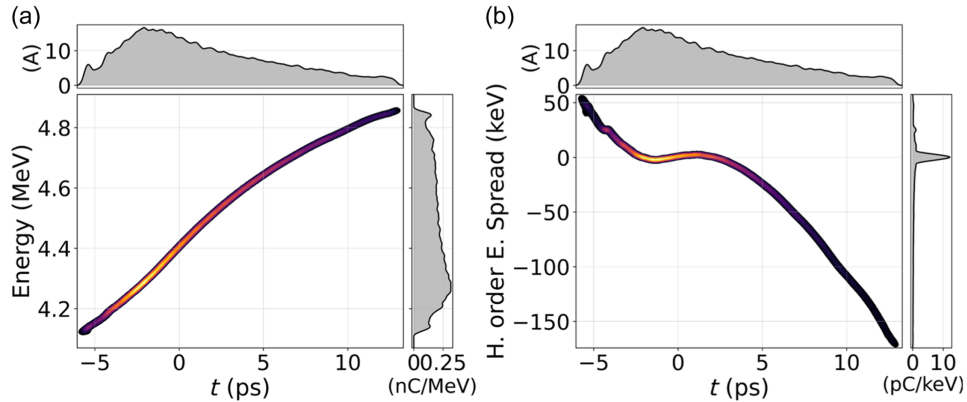


FIG. 16. (a) Bunch energy and (b) higher-order energy spread at the booster entrance.

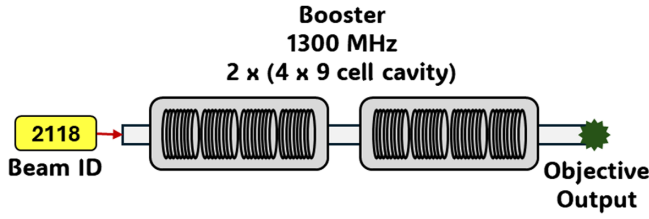


FIG. 17. Further acceleration of the bunch until it reaches the emittance-dominated regime. No optimization is performed at this stage. The two additional booster cryomodules operate on crest.

an increase in bunch energy during compression, as shown in Fig. 16(a). Since the compression does not proceed linearly, the charge distribution develops a peak at the head of the bunch and a long tail, as shown in Fig. 16(b). The resulting rms higher-order energy spread is 38.4 keV, and the peak current reaches 17.3 A.

The bunch was then further accelerated in an individual simulation using two additional cryomodules, as depicted in Fig. 17. The cavities in both cryomodules were used on crest, with an on-axis peak E-field of 30 MV/m.

Figure 18 shows the bunch energy and higher-order energy spread profiles after further acceleration at the end of the booster as shown in Fig. 17.

On-crest acceleration results in a reverse U-shaped longitudinal phase space, as the second- and fourth-order terms dominate the energy gain as described in Appendix B 1. Although the majority of the charge is concentrated at the head of the bunch, the presence of a long tail leads to an additional increase in the higher-order energy spread during acceleration, since it cannot be fully preserved, in contrast to design-I. As a result, the rms higher-order energy spread increases to 50.9 keV.

The normalized projected, core emittances, and bunch duration along the beamline are shown in Fig. 19.

The bunch duration, initially 96.1 ps at the gun exit, was compressed to 17.2 ps, corresponding to a compression factor of 5.6. The normalized projected and core emittances at the compensation point downstream of the gun were

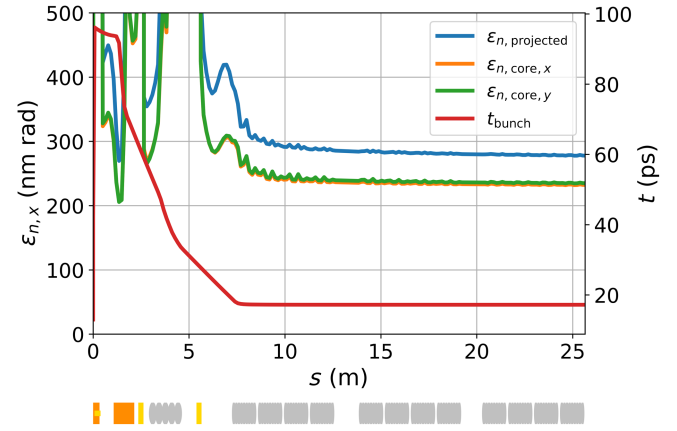


FIG. 19. Evolution of the normalized projected emittance, horizontal and vertical core emittances, and bunch duration along the design-II beamline.

422.9 and 323 nm rad, respectively. Although emittance increased at the prebuncher and buncher cavity exits due to rf-induced correlations and mismatches, the solenoids provided effective emittance compensation and injection into the booster. As a result, the final emittance values were reduced to 278 and 233 nm rad, respectively.

Figure 20 shows the horizontal and vertical phase spaces at the end of the injector, with the core highlighted in both planes.

The axial symmetry between the horizontal and vertical planes was preserved thanks to the use of two-stage rf compression, in contrast to the phase space distortions observed at the end of the magnetic chicane in design-I. As a result, the difference between the core emittance values in the horizontal and vertical planes remained negligible.

Figure 21 presents the horizontal and vertical slice emittances along the bunch, shown together with the one-dimensional current profile.

Although the slice emittance varies by approximately 50 nmrad across the central region of the bunch, it increases by up to a factor of 2 in the tail. This behavior is attributed to the long, low-current tail resulting from the

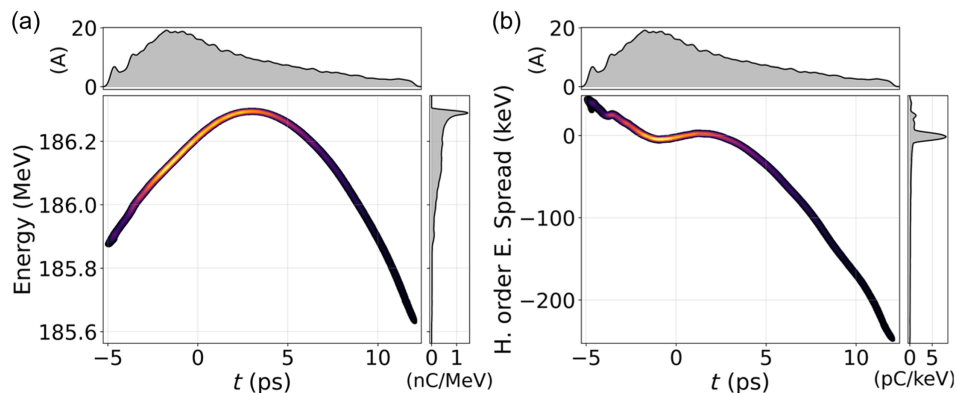


FIG. 18. (a) Bunch energy and (b) higher-order energy spread at the booster exit.

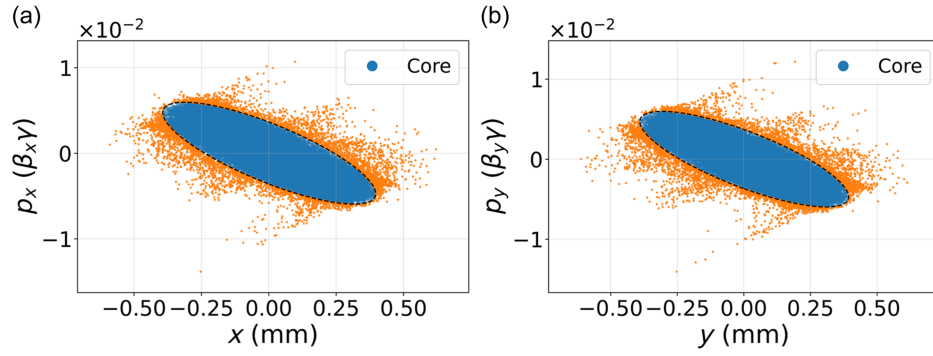


FIG. 20. Horizontal and vertical phase spaces after the booster.

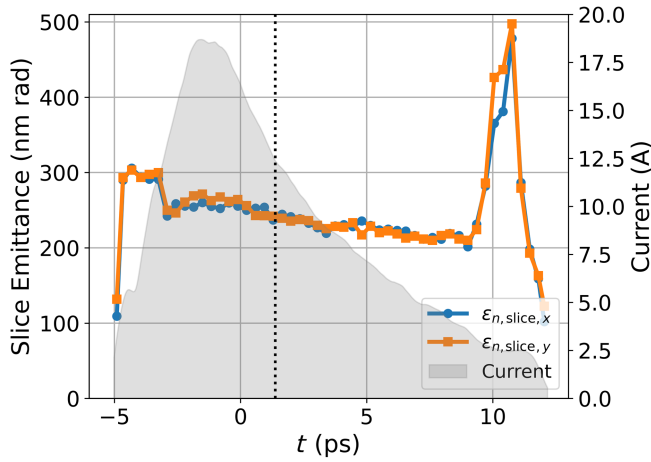


FIG. 21. Horizontal and vertical slice emittances along the bunch, shown together with the final 1D current profile at the end of the booster.

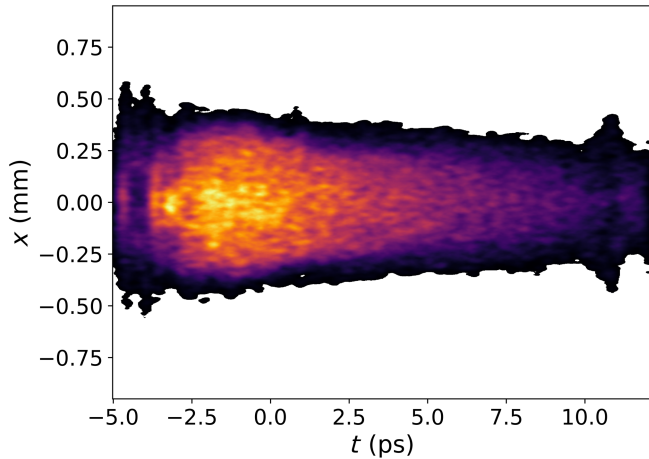


FIG. 22. Beam projection in the horizontal-longitudinal plane. The bunch exhibits an asymmetric profile with the peak current density concentrated at its head.

highly skewed current profile—a characteristic drawback of two-stage rf compression. The final peak current achieved is 18.7 A. Due to the asymmetric shape of the bunch, the weighted mean of the charge distribution is offset from the position of the peak current, highlighting the distortion introduced by the compression scheme.

The beam projection is shown in Fig. 22, where the current density is also illustrated along the bunch.

The bunch exhibits a highly asymmetric longitudinal structure, with the highest current density concentrated near the head, where the transverse beam size is also larger. The tail extends significantly and, unlike in design-I, contributes a noticeable amount to the overall current density, even though the local charge density remains lower than at the head. This broader current density distribution is a direct consequence of the nonlinear compression dynamics. Nevertheless, the achieved peak current is higher than that obtained in design-I for similar final bunch durations, approximately 17 ps, indicating a more aggressive compression in design-II.

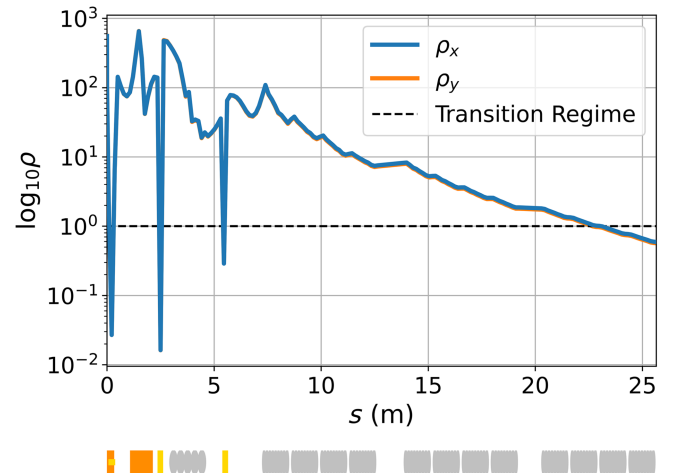


FIG. 23. Evolution of the laminarity parameter along the design-II beamline.

Figure 23 shows the evolution of the laminarity parameter along the design-II beamline. In this case, the transition to the emittance-dominated regime occurs later in the beamline, during acceleration in the third cryomodule, where the beam energy reaches approximately 150 MeV. At the injector exit, the beam reaches a final energy of 187 MeV, confirming that the bunch is emittance dominated and suitable for injection into the main linac.

IV. HIGH-ENERGY BEAMLINE

The main linac section accelerates the bunch from the injector up to a final beam energy of 8 GeV [9] in the baseline design of the UK XFEL. It consists of 73 cryomodules, in which nine-cell 1.3 GHz TESLA-type SRF cavities provide the acceleration. One of the main challenges for beam transport through the main linac is preserving the low beam emittance and energy spread provided by the injector in the presence of collective effects, due to the stringent electron beam quality requirements imposed by the FEL. Moreover, the bunch length must be compressed by approximately two orders of magnitude relative to its value at the end of the injector to reach peak current levels in the kA range; this is commonly achieved by using magnetic bunch compression in two or more stages.

The magnetic compression scheme in the baseline design of the high-energy linac employs two asymmetric five-dipole magnetic chicanes distributed along the main linac, in place of the conventional symmetric four-dipole (C-shaped) configuration. The choice of an asymmetric five-dipole geometry is motivated by theoretical and numerical studies, which demonstrate its ability to nearly cancel the coherent synchrotron radiation (CSR)-induced kicks imparted to the bunch during compression, thereby improving the preservation of beam brightness [28]. Since the longitudinal phase space must be linearized before the first compression stage, a higher-harmonic 3.9 GHz rf cavity operating at the third harmonic of the main linac frequency is included. A detailed description of the main linac and bunch compression design for the UK XFEL will be presented in a future publication.

The two injector designs described above are compared in terms of final beam quality after full acceleration and compression along the main linac, to elucidate their differences and assess their suitability for meeting the XFEL requirements. Representative bunches—identified by their simulation IDs in the previous sections—with similar peak currents (16.0 and 18.7 A) were tracked through the main linac and bunch compressors using the ELEGANT code [29], including CSR effects, longitudinal space charge, and geometric wakefields from the rf structures. The objective is to evaluate how well each injector configuration satisfies the beam quality specifications required across the FEL lines envisioned for the UK XFEL. This is done by comparing key parameters such as the ability to sustain a relatively flat 2 kA current profile and to preserve a normalized emittance of approximately 350 nm rad after

compression and acceleration through the main linac. Figure 24 presents the slice properties and phase space distributions of the compressed 8 GeV bunch at the end of the main linac for representative bunches from both injector designs. An overcompressed case from design-II, shown in the bottom row, is also included to support further discussion on the implications of eliminating the long tail along the main linac.

The results of the main linac tracking for the bunch delivered from the design-I are shown in Figs. 24(a)–24(c). The bunch is compressed down to ≈ 116 fs, corresponding to a compression factor of ≈ 145 . The initial slice emittance shown in Fig. 11 is almost fully preserved through the main linac. Although a noticeable horizontal emittance dilution is observed at the head of the bunch—likely due to incomplete cancellation of CSR effects, as shown in Fig. 24(a)—the current in that region remains relatively low compared to the peak current of approximately 2.5 kA. Consequently, that portion of the bunch is not expected to contribute significantly to the FEL lasing process. A similar conclusion applies to the tail of the bunch, where the current is also low despite a smaller emittance growth. The core of the bunch exhibits a relatively flat current profile of around 2 kA, with a mean relative slice energy spread around 4×10^{-4} , as shown in Fig. 24(b). The longitudinal phase space depicted in Fig. 24(b) shows clear evidence of the microbunching instability [30–33]. Mitigating the effect of microbunching, through the use of a laser heater [30,34], transverse optics control [35], or another method, will be the subject of a future study. Figure 24(c) illustrates the longitudinal-transverse correlation of the charge distribution. A significant portion of the bunch is confined symmetrically within a duration of approximately 80 fs (between -45 and 35 fs). The effect of horizontal emittance dilution at the head of the bunch observed in Fig. 24(a) is also evident as an increase in the transverse beam size in that region in Fig. 24(c).

The results from the design-II injector configuration are shown in Figs. 24(d)–24(f). For this design, the rf phases of the linac and linearizer cavities were adjusted with respect to design-I in order to achieve a similar peak current. The horizontal and vertical emittances are both smaller and exhibit less dilution at the head of the bunch compared to those in design-I. The initial asymmetry in the current profile arising due to the two-stage rf compression is preserved, as shown in Fig. 24(d). In order to maintain the same linear energy chirp as in the design-I case, the asymmetry in the current profile cannot be eliminated, which results in a tail in the bunch extending up to 200 fs, which is approximately 4 times longer than the concentrated charge distribution at the head of the bunch as shown in Fig. 24(e). The mean relative energy spread at the head of the bunch is smaller than the value of 4×10^{-4} obtained for the core of the bunch in design-I. Furthermore, the asymmetry in the current profile leads to an imperfect

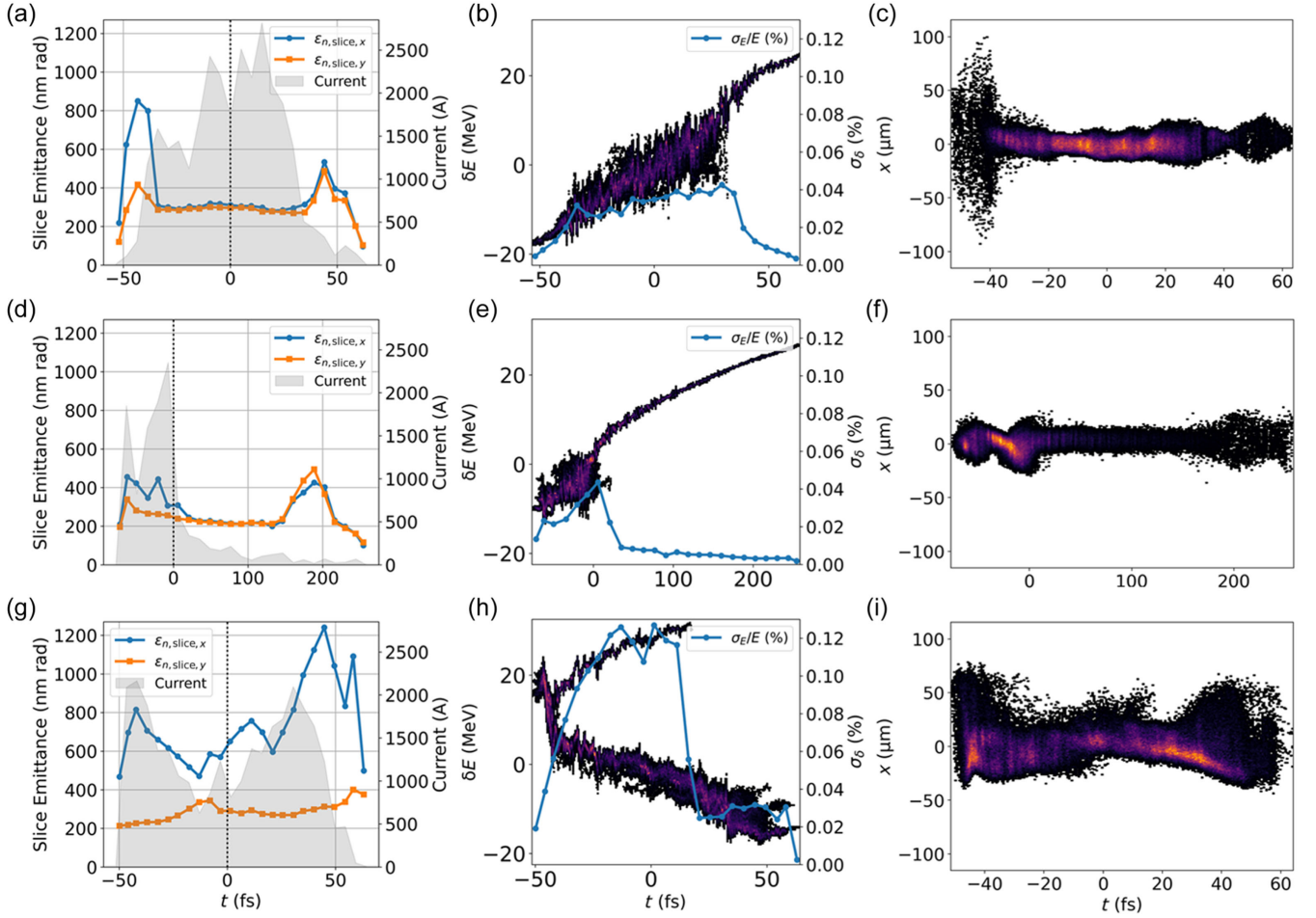


FIG. 24. Slice properties and phase spaces of the compressed 8 GeV beam at the end of the main linac: (a)–(c) using design-I optimization parameters; (d)–(f) using design-II optimization parameters; (g)–(i) design-II optimization parameters, overcompressed.

cancellation of CSR effects, and therefore a slight increase in horizontal slice emittance, and a considerable asymmetry as demonstrated in the beam projection shown in Fig. 24(f). While the length of the bunch tail could be reduced by adjusting the phasing of the accelerating cavities, this came at the cost of increasing the final bunch compression factor and a further degradation of the beam quality beyond the acceptable range required for the FEL. The final bunch duration is 355 fs, while the charge distribution confined to the head of the bunch (between -70 and 50 fs) has a 120 fs bunch duration. Given that only the head of the bunch is suitable for the lasing process in the design-II case, the long tail may require collimation. However, this is not an optimal solution, as it compromises the goal of utilizing the full bunch charge and may lead to issues with radiation protection. As an alternative, a modified compression scheme was explored in which the bunch is overcompressed to fold the tail back onto the head. Figures 24(g)–24(i) show the results of this overcompression scenario for the design-II bunch. While this approach achieves a shorter bunch duration of 135 fs and a more uniform charge distribution along the bunch as shown in

Fig. 24(i), it also causes emittance dilution, particularly in the horizontal plane as shown in Fig. 24(g). Additionally, the slice energy spread increases by a factor of 4 compared to the two other cases, as demonstrated in Fig. 24(h). This is primarily due to the overlap of high-energy tail particles with lower-energy particles at the head of the bunch—a natural outcome of the overcompression process. The results clearly demonstrate that overcompression is not a viable method, as it leads to significant emittance growth and energy spread beyond FEL tolerances. Consequently, it is not considered a suitable option for mitigating the long tail and hence is excluded from further performance comparisons.

A direct comparison of the normalized 6D brightness at the end of the main linac is presented in Fig. 25 for both baseline injector configurations, using the slice parameters obtained in Figs. 24(a), 24(b), 24(d), and 24(e). The relative energy spread (σ_E/E) is normalized to 0.1%, and the brightness is reported in units of $\text{A}/\text{m}^2/0.1\%$ to ensure consistency with the literature [36].

Design-I yields a peak brightness of approximately $0.97 \times 10^{17} \text{ A}/\text{m}^2/0.1\%$ close to the bunch centroid. The high-brightness region extends broadly from -40 to $+40$ ps,

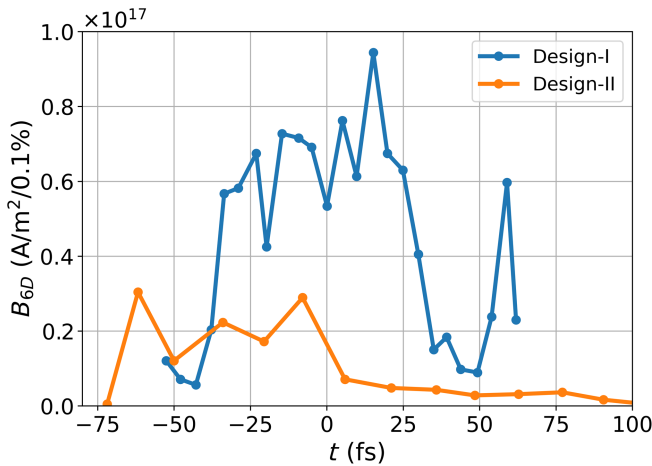


FIG. 25. Normalized 6D brightness expressed in units of $\text{A/m}^2/0.1\%$ using the slice parameters for both baseline injector configurations shown in Figs. 24(a), 24(b), 24(d), and 24(e).

within which $B_{6D,n}$ remains above $0.4 \times 10^{17} \text{ A/m}^2/0.1\%$. This sustained brightness across the core reflects an effective bunch compression and good emittance preservation, rendering the bunch highly suitable for FEL lasing. In contrast, design-II exhibits a substantially lower brightness profile, with a peak value of only $0.29 \times 10^{17} \text{ A/m}^2/0.1\%$, localized in the head of the bunch. The brightness quickly diminishes outside this narrow region and remains below $0.1 \times 10^{17} \text{ A/m}^2/0.1\%$ throughout the rest of the bunch due to the long tail, which limits its FEL applicability. The 6D brightness results highlight that preserving the charge distribution symmetry in the injector leads to a better 6D brightness at the linac exit, directly enhancing FEL gain potential.

A set of different jitter sources was considered in this study for both injector designs, with the analysis focused on evaluating their impact on key beam parameters. The applied jitter levels—gun rf phase jitter (0.0148°), gun voltage jitter ($\pm 0.011\%$), laser timing jitter ($\pm 100 \text{ fs}$), and laser power jitter ($\pm 1\%$)—were observed at the end of each injector beamline [17,37]. It was found that these jitter sources had a negligible impact on the key beam parameters such as horizontal and vertical core emittances, bunch energy, high-order energy spread, peak current, and charge distribution skewness in both cases. However, gun voltage and laser timing jitter resulted in a shift in beam arrival time. The resulting beam arrival-time variation due to gun voltage jitter was 151 fs in design-I and 81 fs in design-II, whereas laser timing jitter led to shifts of 148 and 127 fs, respectively. From the XFEL perspective, such arrival-time variations, which might not be critical at the injector level, could still influence synchronization in downstream sections, particularly in time-resolved experiments. Since jitter can evolve through the machine and may be altered by downstream elements such as bunch compressors; a complete understanding of its effect requires start-to-end jitter

tracking. This is beyond the scope of the current work and will be addressed in future design phases.

V. DISCUSSION

Beyond the achieved beam dynamics performance, several practical and engineering-driven aspects must be addressed in the next stages of development to ensure a successful transition from conceptual design to technical realization.

The relaxed VHF gun geometry, which draws inspiration from the APEX2 design, offers the advantage of higher achievable beam energy at the gun exit due to an extended accelerating gap. However, this comes at the cost of compactness and introduces mechanical integration challenges. In particular, the placement of solenoids within the re-entrant geometry—essential for emittance compensation—must be carefully evaluated during the engineering phase to ensure magnetic field alignment, mechanical stability, and the mitigation of potential multipactor effects without compromising performance.

Regarding the NC rf cavities, the baseline configuration using a single-cell 216.67 MHz prebuncher and a 650 MHz linearizer has proven effective in simulations. However, in practice, it may be necessary to adopt two- or three-cell designs. Multicell cavities reduce peak surface fields to better manage cw heat loads and accommodate additional cooling channels, all while keeping cavity lengths compatible with beamline integration. As such, additional development work will likely be required to adapt the design for experimental implementation without compromising the bunch shaping and chirp control essential to the compression process.

The current magnetic compressor design does not include quadrupoles on either side of the chicane to control the beam optics through the chicane and match the beam to the next section of the accelerator. As a result, the only focusing that acts on the beam is from the dipole edges. Better control of the beam sizes through the chicane may help to mitigate some of the transverse emittance growth. The addition of these matching quadrupoles will be considered in the next stage of the design work.

The merger section, which transports the beam from the low-energy injector into the main linac, has been assumed to be effectively transparent in its impact on beam quality. While this assumption is justified for a well designed, achromatic, and isochronous beamline, careful verification through start-to-end tracking, including 3D space charge and coherent radiation effects, will be required in future work. Any residual dispersion, CSR-induced energy spread, or wakefield effects introduced in this region could degrade the emittance or disturb the longitudinal phase space established during compression.

In the main linac, one of the persistent challenges is the preservation of beam brightness during further acceleration and magnetic bunch compression. The high peak currents

required for FEL operation amplify microbunching instabilities, particularly due to the chirped nature of the bunches exiting the injector. The use of a laser heater system may be essential to suppress these instabilities by increasing the uncorrelated energy spread to a controlled level, thereby reducing gain in microbunching while still meeting the tight relative energy spread requirements—on the order of 1×10^{-4} at the undulator entrance. Furthermore, simulations suggest that replacing the chicane with an arc-based compressor is an attractive alternative option, both in terms of mitigating the microbunching instability, and for producing a large central current spike in the electron bunch. A detailed discussion on the optimization of the main linac, and a consideration of the bunch compression options, are beyond the scope of this paper and will be presented in a future publication.

Finally, beam transport through the spreader lines that direct electron bunches to the various FEL beamlines introduces an additional stage where emittance growth might occur due to CSR and residual dispersion. Ensuring that beam quality is maintained not only through the injector and linac but also into the final delivery systems is critical to guaranteeing reliable FEL gain across the photon beamlines envisioned for the UK XFEL.

VI. CONCLUSION

In this study, the conceptual design and comparative performance evaluation of two injector configurations are developed for the UK XFEL to produce high-brightness electron bunches optimized for subsequent acceleration in the main linac up to 8 GeV. Both designs were optimized at a bunch charge of 150 pC, a representative working point that balances FEL performance requirements with preservation of beam quality during compression. Emphasis was placed on achieving sub-20 ps bunch durations at the injector exit while addressing key performance metrics.

At the injector exit, design-I achieves a bunch duration of 16.9 ps and design-II 17.0 ps, with corresponding peak currents of 16.0 and 18.7 A. Design-I yields 285 nm rad horizontal and 268 nm rad vertical transverse core emittance, an average rms energy spread of approximately 2.0×10^{-4} , and a nearly symmetric longitudinal charge distribution with a skewness of 0.08. In contrast, design-II attains lower transverse emittances of 233 nm rad in both horizontal and vertical directions, an rms energy spread below 0.5×10^{-4} , but exhibits significant longitudinal asymmetry indicated by a skewness of 0.7.

Start-to-end simulations through the main linac further highlight the implications of these injector differences. Both configurations achieve slice energy spreads around 4.0×10^{-4} at the linac exit, and meet the XFEL slice emittance requirement of less than 350 nm rad. Design-II achieves slightly lower minimum slice emittance values, reaching approximately 200 nm rad, compared to around 250 nm rad for design-I. Peak currents remain above 2 kA

in both cases, satisfying UK XFEL operational requirements. However, design-II experiences pronounced tail elongation and degraded slice quality due to its initial asymmetry, severely limiting the effective lasing region. Conversely, design-I maintains a compact and symmetric longitudinal charge distribution throughout the acceleration and compression processes, preserving uniform slice quality and emittance. A quantitative comparison of normalized 6D brightness at the main linac exit reinforces these findings. Design-I achieves a peak normalized brightness of approximately 0.97×10^{17} A/m²/0.1%, sustained across a broad central region of the bunch. In contrast, design-II reaches a significantly lower peak brightness of 0.29×10^{17} A/m²/0.1%, with brightness rapidly diminishing toward the tail region.

These results demonstrate that, although both injector designs meet baseline XFEL requirements, preserving the symmetry of the longitudinal charge distribution is essential to achieving superior FEL performance. Recovering from the longitudinal asymmetry introduced in earlier stages proves challenging without significant degradation of beam quality. Considering the combined injector and main linac results, design-I emerges as a robust candidate for high-brightness, high-repetition-rate XFEL injectors, offering an optimal balance of beam brightness, compressibility, and longitudinal phase space quality to meet the stringent requirements of XFEL operation.

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DATA AVAILABILITY

The data that support the findings of this article are not publicly available because of legal restrictions preventing unrestricted public distribution. The data are available from the authors upon reasonable request.

APPENDIX A: RF CAVITY DESIGNS

Appendix A shows the CST [38] optimization of the rf cavities used during the low-energy injector design optimization. Appendix B reviews the fundamentals of longitudinal bunch compression schemes, both for rf and

magnetic compression schemes. Appendix C discusses the key beam quality metrics used either as objectives in the multiobjective optimization simulations or as figures of merit for the different design options.

The optimization of both the single-cell NC and the five-cell SRF cavities is presented in this appendix. All cavity optimizations were carried out using CST Microwave Studio's eigenmode solver, and the field distributions shown were normalized to a stored energy of 1 J.

1. Single-cell NC cavities

To assess the influence of rf frequency on bunch compression quality, three single-cell nose-cone cavities with identical geometries were designed at 216.67, 650.0, and 1300 MHz based on the reference design of Ref. [39]. The reference cavity was first validated at 1.3 GHz by reproducing its field profile, quality factor, and shunt impedance. This validated geometry was then scaled to the three target frequencies and analyzed. Figure 26

illustrates the electric and magnetic field distributions for the 650 MHz cavity, which serves as the linearizer in both design-I and design-II.

The dissipated power was calculated to be 12.68 kW, and the longitudinal peak electric field was estimated at 2.64 MV/m, in agreement with Ref. [40].

2. Five-cell SRF cavity

To accommodate the long bunches emerging from the injector, a 650 MHz booster structure was adopted. The booster is a five-cell elliptical SRF cavity which originated from the nine-cell, 1.3 GHz TESLA design [12]. Figure 27 shows the longitudinal electric field of five-cell booster.

Eigenmode simulations yield an R/Q of 558Ω (the shunt impedance per unit quality factor) and a geometry factor 272Ω , indicating efficient acceleration with controlled surface losses. Surface-field ratios of $E_{\text{peak}}/E_{\text{acc}} = 2.0$ and $B_{\text{peak}}/E_{\text{acc}} = 4.74 \text{ mT}/(\text{MV}/\text{m})$ ensure operation below field emission and quench thresholds, where E_{peak}

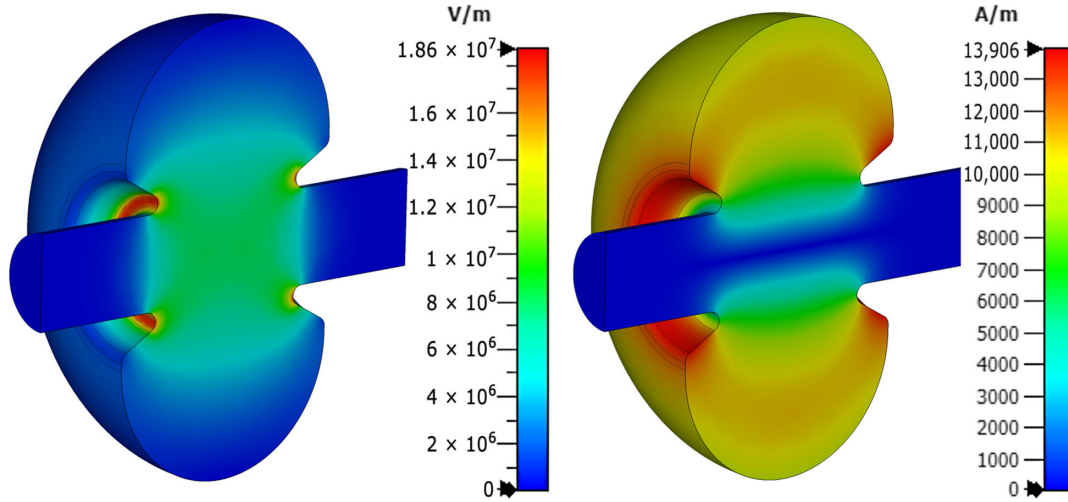


FIG. 26. Electric and magnetic fields for the 650 MHz NC rf cavity.

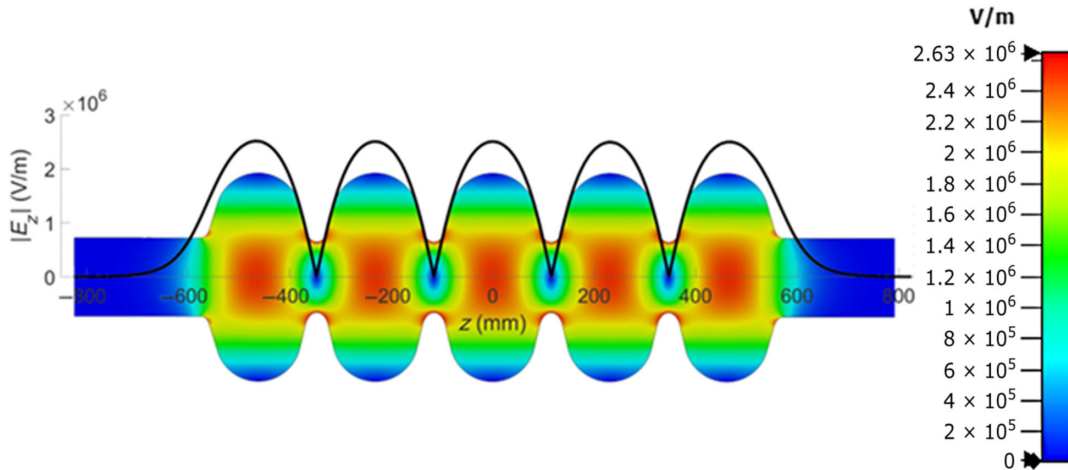


FIG. 27. Five-cell booster cavity longitudinal E-field.

and B_{peak} are the maximum local electric and magnetic fields on the cavity surface, and E_{acc} is the average accelerating gradient. The five cells exhibit 99% field flatness for the longitudinal field normalized to 1 J of stored energy.

APPENDIX B: LONGITUDINAL BUNCH COMPRESSION

To enable effective injection into the main linac, the bunch duration is typically expected to be shorter than 20 ps, which corresponds to approximately 10° of the 1.3 GHz rf wavelength—a commonly used rule of thumb. Longer bunches mitigate emittance growth at the gun but require subsequent compression and acceleration with preserved transverse emittance. This section provides an overview of rf and magnetic bunch compression schemes, both of which are utilized in the alternative injector design options explored in this study.

1. rf compression

rf compression is a key technique for shortening the electron bunch duration (temporal length), particularly at low energies, by imparting a correlated energy spread (or energy chirp) along the bunch. The effectiveness of rf compression is critically governed by the longitudinal dynamics of the particles within the rf cavity. The position of each particle along the bunch, corresponding to a specific rf phase, determines the energy deviation it experiences in the cavity. The energy deviation of a single charged particle in an rf standing-wave cavity can be defined as

$$\Delta E(z) = eV \cos(kz + \phi), \quad (\text{B1})$$

where e is the charge of the particle, V is the peak rf voltage that the particle experiences in the cavity, k is the wave number, z is the longitudinal position along the cavity axis, and ϕ is the phase of the particle in the rf field. Considering that Eq. (B1) applies to all charged particles within a bunch, the relative energy deviation (spread) of each particle in the cavity can then be written as

$$\delta(z) = \frac{\Delta E(z)}{E_0} \approx \frac{E(z) - E_0}{E_0} = \frac{eV}{E_0} \cos(kz + \phi), \quad (\text{B2})$$

which explains how the energy of a particle depends on its longitudinal position within the bunch, where E_0 is the mean energy of the bunch. The relative energy spread, assuming that $kz \ll 1$ can be expanded using a Taylor series, is

$$\delta(z) = \frac{eV}{E_0} \left[\cos(\phi) - kz \sin(\phi) - \frac{(kz)^2}{2} \cos(\phi) + \frac{(kz)^3}{6} \sin(\phi) + \frac{(kz)^4}{24} \cos(\phi) + \dots \right], \quad (\text{B3})$$

which reveals the linear and nonlinear contributions. In particular, when the cavity operates on crest (i.e.,

$\phi \rightarrow 0^\circ, 180^\circ$), the terms multiplied by $\sin(\phi)$ become negligible, and Eq. (B3) simplifies to

$$\delta(z) = \frac{eV}{E_0} \left[\cos(\phi) - \frac{(kz)^2}{2} \cos(\phi) + \frac{(kz)^4}{24} \cos(\phi) \right], \quad (\text{B4})$$

where the quadratic (second) and quartic (fourth) orders dominate, leading to a U-shaped phase space curvature. Conversely, when the cavity operates at zero crossing (i.e., $\phi \rightarrow 90^\circ, 270^\circ$), the terms multiplied by $\cos(\phi)$ vanish, yielding

$$\delta(z) = \frac{eV}{E_0} \left[-kz \sin(\phi) + \frac{(kz)^3}{6} \sin(\phi) \right], \quad (\text{B5})$$

where linear (first) and cubic (third) orders govern the relative energy spread, leading to an S-shaped phase space curvature. Figure 28 illustrates how particles within the bunch at different longitudinal positions—corresponding to different rf phases—experience varying energy deviations.

Depending on the chosen rf phase, one of the two rf compression techniques—ballistic bunching or velocity bunching—can be employed. In ballistic bunching, the bunch passes through an rf cavity operated at the zero-crossing phase, where no net energy gain occurs but a predominantly energy chirp is imparted. The tail of the bunch gains more energy than the head, leading to bunch compression in the subsequent drift. In contrast, velocity bunching is achieved by injecting the bunch at an off-crest phase between the “acceleration” and “compression”

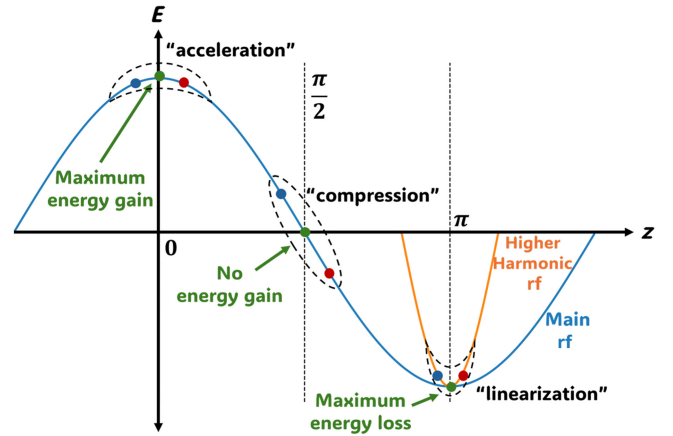


FIG. 28. Key rf operating regions: on crest, where the bunch experiences maximum energy gain; zero crossing, where no net energy gain occurs but an energy chirp is introduced; and negative on crest, where the bunch undergoes maximum energy loss. The negative on-crest region is commonly exploited to linearize the longitudinal phase space by using a higher-harmonic cavity—most often the third harmonic as illustrated in the figure—to compensate for rf-induced curvature as described in Eq. B(3).

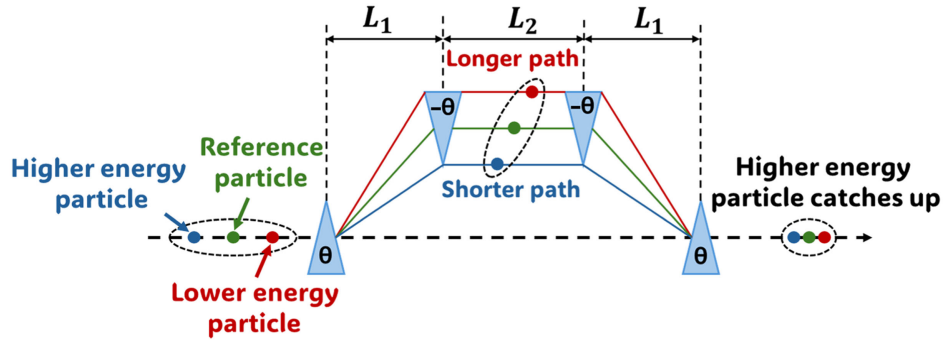


FIG. 29. C-shaped symmetric magnetic chicane used for bunch compression. The layout illustrates the beam trajectory along with three representative particles at the head, center, and tail of the bunch to demonstrate the energy-dependent path length differences and bunch compression dynamics [6].

phases. In this case, the bunch is primarily compressed within the rf structure itself, as tail particles—initially at lower energies—gain velocity and catch up with the head during acceleration. The effectiveness of each method depends on factors such as the initial bunch energy, rf frequency, and the available drift length following the rf cavity. One should note that nonlinear rf contributions can distort the longitudinal phase space and, consequently, the compressed bunch profile. Higher-harmonic linearization is therefore an effective method for mitigating these higher-order distortions. In this work, higher-harmonic linearization is implemented using a cryomodule of four nine-cell, 1.3 GHz TESLA-type superconducting cavities—operating as the second harmonic of the 650 MHz injector booster—thereby eliminating the need for an additional klystron.

2. Magnetic compression

Magnetic compression employs dipole magnets to introduce energy-dependent path length differences for the particles within the bunch. The particle energy is not affected by the choice of chicane geometry, such as C-shape, S-shape, arc, or double-bend, in cases where synchrotron radiation is negligible. However, the path length varies with particle energy, enabling compression for energy-chirped bunches. Figure 29 shows a C-shaped symmetric chicane, one of the most common magnetic compression schemes employed in accelerator facilities.

Considering a bunch accelerated and given sufficient chirp before the chicane, the linear compression factor can be defined by

$$C = \frac{1}{|1 + hR_{56}|}, \quad (\text{B6})$$

where h is the linear chirp with units of m^{-1} , and R_{56} is the transfer matrix element that quantifies the dependence of a particle's longitudinal position on its energy (momentum) deviation defined in meters. Equation (B6) allows the calculation of R_{56} for a given compression factor and an adjusted linear chirp after acceleration and linearization as

described in the previous section. Therefore, once the R_{56} is theoretically found, a C-shaped symmetric chicane can be placed onto the beamline for magnetic compression by matching this calculated R_{56} with

$$R_{56} \cong -2\theta_0^2 \left(L_1 + \frac{2}{3}L_2 \right), \quad (\text{B7})$$

where θ_0 is the bending angle, L_1 and L_2 are the distances between the first and second dipoles and between the second and third, respectively. Magnetic compression is generally employed at beam energies above 100 MeV to ensure that the bunch is in the emittance-dominated regime, where space charge forces become negligible. This principle is discussed in more detail in Appendix C3.

APPENDIX C: OPTIMIZATION PARAMETERS

The multiobjective optimization of alternative low-energy beamline designs employed four key performance metrics—transverse core emittance, skewness of the longitudinal charge distribution, the laminarity parameter, and bunch duration—to evaluate and improve overall injector performance.

1. Transverse core emittance

Using the rms normalized emittance of the full bunch as an optimization objective tends to overestimate the impact of outer particles and slice-to-slice rotations in the transverse phase space. Conversely, the average slice emittance, calculated over longitudinal slices, underestimates the collective beam behavior by neglecting global correlations across the bunch. As a result, neither metric alone sufficiently captures the true transverse beam quality and effectively guides the optimization toward an optimal transverse emittance solution. A more accurate characterization requires a slice-informed yet globally aware approach that selectively excludes particles contributing to spurious emittance growth.

To address this, a core transverse emittance is defined, offering a more representative and physically meaningful measure of transverse phase space quality. In practice, the core is typically defined to include 95.45% of the total bunch charge. In this work, the Mahalanobis distance-based method [41] is employed to determine the elliptical boundary of the core in transverse phase space and to identify the subset of particles used for emittance evaluation. The approach leverages the full two-dimensional transverse phase space (x, p_x) and explicitly incorporates the beam centroid, assuming an axisymmetric transverse distribution. For each particle, the deviation vector is defined as

$$\Delta \mathbf{x}_i = \begin{pmatrix} x_i - \bar{x} \\ p_{x,i} - \bar{p}_x \end{pmatrix}, \quad (\text{C1})$$

and its squared Mahalanobis distance is given by

$$D_i^2 = \Delta \mathbf{x}_i^T \Sigma_x^{-1} \Delta \mathbf{x}_i, \quad (\text{C2})$$

for

$$\epsilon_{n,\text{core},x} = \sqrt{\det \Sigma_x} = \sqrt{\langle x^2 \rangle \langle p_x^2 \rangle - \langle x p_x \rangle^2}. \quad (\text{C3})$$

By sorting the particles in order of increasing D_i^2 and accumulating their charge until 95.45% of the total is reached, this approach defines an elliptical core that captures the phase space directionality. The use of the defined beam centroid as a reference ensures that any rotation or tilt in the phase-space ellipse is taken into account, which is critical for beam matching, optics design, and compensation for misalignment or chromatic effects. Moreover, under ideal slice alignment conditions, the defined core emittance converges closely to the average slice emittance. By fully incorporating the covariance structure of the beam, this method provides a directional core definition aligned with the principal axes of the transverse phase-space ellipse. As a result, no additional correction using Twiss parameters is required, unlike other techniques utilizing the convex hull method [42]. This robust approach ensures a core definition that reflects intrinsic beam dynamics, thus delivering improved accuracy and valuable insights for transverse beam dynamics and optimization.

2. Skewness of the longitudinal charge distribution

When evaluating longitudinal beam quality, particularly in the context of bunch compression, it is essential to account for both the energy spread and higher-order energy correlations, as these factors limit the achievable bunch duration and shape the longitudinal charge distribution. To achieve optimal compression, nonlinear rf-induced distortions must be minimized. Additionally, controlling the charge distribution along the bunch is critical to mitigating head and tail instabilities during acceleration.

To address these aspects, the skewness of the longitudinal charge distribution is introduced as an optimization parameter. For a bunch of particles with longitudinal positions z_i and corresponding weights q_i , the weighted mean μ , which corresponds to the charge-weighted centroid of the bunch, is defined as

$$\mu = \frac{\sum_i z_i q_i}{\sum_i q_i}. \quad (\text{C4})$$

The weighted variance σ^2 , which measures the spread (i.e., second central moment) of particle positions about the centroid, is given by

$$\sigma^2 = \frac{\sum_i (z_i - \mu)^2 q_i}{\sum_i q_i}, \quad (\text{C5})$$

The weighted third central moment M_3 , which quantifies the asymmetry of the distribution about the mean, is defined as

$$M_3 = \frac{\sum_i (z_i - \mu)^3 q_i}{\sum_i q_i}. \quad (\text{C6})$$

The skewness S is then given by

$$S = \frac{M_3}{\sigma^3}. \quad (\text{C7})$$

A skewness of zero indicates a perfectly symmetric charge distribution, while nonzero values signify asymmetry. In this work, minimizing the absolute value of skewness is used as a proxy to reduce higher-order energy spread and improve the quality of the longitudinal phase space during the optimization.

3. Laminarity parameter

To isolate the intrinsic beam dynamics driven by self-interactions, the external focusing and acceleration terms are often neglected. Under these conditions, the beam envelope is governed by the simplified equation:

$$\sigma'' - \frac{\kappa_s}{\sigma \beta^3 \gamma^3} - \frac{\epsilon_n^2}{\sigma^3 \beta^2 \gamma^2} = 0, \quad (\text{C8})$$

where σ is the rms beam size, κ_s is the beam perveance, β and γ are the normalized velocity and Lorentz factor of the beam, and ϵ_n is the normalized emittance [43]. The first term represents the curvature of the beam envelope, indicating changes in its slope. The second term corresponds to the defocusing influence of space charge, and the third term accounts for the internal pressure due to emittance.

The beam perveance is defined as

$$\kappa_s = \frac{\hat{I}}{2I_A}, \quad (\text{C9})$$

where $\hat{I}$ is the peak current and I_A is the Alfvén current, approximately 17 kA. From Eq. (C8), two distinct beam transport regimes can be identified: a space charge-dominated regime and an emittance-dominated regime. A beam is considered space charge dominated when collective effects due to space charge significantly outweigh those due to emittance. The relative importance of space charge can be quantified by the laminarity parameter [44], ρ , which is defined as

$$\rho = \frac{\text{Space charge force}}{\text{Emittance pressure}} = \frac{\kappa_s \sigma^2}{\epsilon_n^2 \beta \gamma}. \quad (\text{C10})$$

The beam is in the space charge-dominated regime for $\rho > 1$, where collective forces govern beam dynamics. Conversely, when $\rho < 1$, the beam is in the emittance-dominated regime, and space charge effects can be neglected as internal emittance pressure becomes dominant. In this work, the laminarity parameter is evaluated to verify that the beam transitions into the emittance-dominated regime before entering the main linac. This condition ensures that space charge effects become negligible during downstream acceleration, thereby preserving beam quality and avoiding additional emittance growth or phase space distortions.

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