Closed-Form and Machine-Learned Surrogates for Determining Impurity Limits and Operating Windows in Low-Activation Fusion Materials

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Deuterium-tritium fusion is often described as intrinsically low-waste, however ensuring that fusion components meet low-level waste (LLW) acceptance criteria under U.S. regulatory frameworks (10 CFR 61) requires coordinated control of impurity content and operating conditions. This study develops an accelerated surrogate framework to support that task by linking isotope-resolved waste disposal rating (WDR_i) to impurity concentration, major radius, fusion power, and operating time across a generic tokamak parameter sweep. A closed-form ordinary differential equation (ODE) for WDR_i is fit to activation-derived reference data at 100 years cooling, with the goal of enabling rapid estimation of the operating characteristics required to keep the total waste disposal rating from contributing isotopes (WDR) below unity, or conversely, the impurity levels allowable for a given operating point. The ODE reproduces the dominant behavior across most cases and provides an interpretable screening tool, but residual analysis reveals structured radius, impurity, and blanket-dependent bias, indicating that a single fixed closed-form expression is too rigid to fully capture all production and depletion patterns under one roof. This limitation is especially evident in specific impurity-blanket combinations, such as Ho in RAFM-Li4SiO4. To address this, we present a Kernel Ridge Regression (KRR) surrogate trained directly on operating and material descriptors, testing whether a more flexible data-driven model can better encode these patterns while preserving the rapid evaluation needed for impurity specification and design-space exploration.

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