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Materials Data Analytics for Advanced Alloy Development: 9-12{\%}Cr Steel. VYACHESLAV ROMANOV, National Energy Technology Lab, NARAYANAN KRISHNAMURTHY, Univ of Pittsburgh, JEFFREY HAWK, National Energy Technology Lab — The project goal is to develop expertise in domain-guided statistical design for optimal manufacturing, computational materials engineering, with uncertainty quantification to support decision-making, and additional scientific insight into complex, noisy, high-dimensional, and high-volume data sets from experiments and simulations. Predictive models will be validated against experimental data. Data entries in the analyzed 9-12{\%}Cr Steel dataset for iron base alloy compositions (\textgreater 80), processing parameters, results of strength and creep tests were arranged in 47 columns by 2800 rows. Detailed microstructural information was not available. Complexity of the phase transformations and microstructure evolution in multi-component (21 chemical elements) alloys, with major influence on mechanical properties, leads to inefficiency in direct application of unbiased linear regression across the entire data space. To address the non-linearity, without using microstructure data, analyses of tensile and creep data were carried out in composition-based clusters. Partitioning revealed the biased nature of available alloy datasets, with implied "rules of thumb" in design practices; processing and test temperatures effects on the phases and mechanical properties are the major contributors and need to be modeled first, before searching for minor effects of the composition variations; Mn and C (and to a lesser extent, N) are global variables, while other elements tend to produce local (non-linear, cluster-centered) dependencies.

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