Bimodal impact strength distribution in HDPE composites: formulational effects and Bayesian inference. Appendix A.

Abstract

A bimodal impact strength distribution was found in notched impact specimens of HDPE composites with calcium carbonate, carbon black, SEBS and stabilisers. The bimodal distribution was only found at moderate-to-high calcium carbonate loadings, with the likelihood of low impact strength increasing with increasing stabiliser loading and decreasing with increasing SEBS/CB masterbatch loading. Bayesian methods were used first to confirm bimodality and then to investigate the effects of formulation on the performance of the system, based on a hierarchical model with quadratic and interactive terms and switching based on the sampling of a Bernoulli distribution with a logistic regression informing the probability of high or low impact strength. The results are contextualised through micrograph fractography and, briefly, differential scanning calorimetry. Results are also reported for unnotched impact tests, with negative correlations for impact strength with calcium carbonate and stabilisers, a positive correlation with SEBS/CB and interactive effects.

Keywords: Bayesian inference, polymer composites, bimodal, impact strength, fractography

A1. Notched impact strength

A1.1. 30CC

A1.1.1. Bimodality test

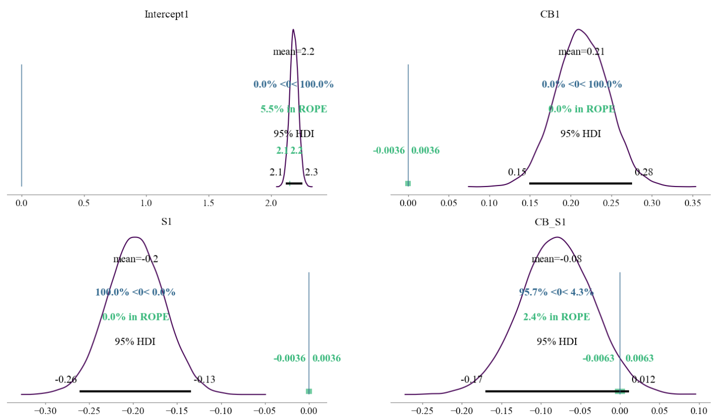

Figure A1: Posterior parameter distributions: notched impact strength; single linear model; 30CC.

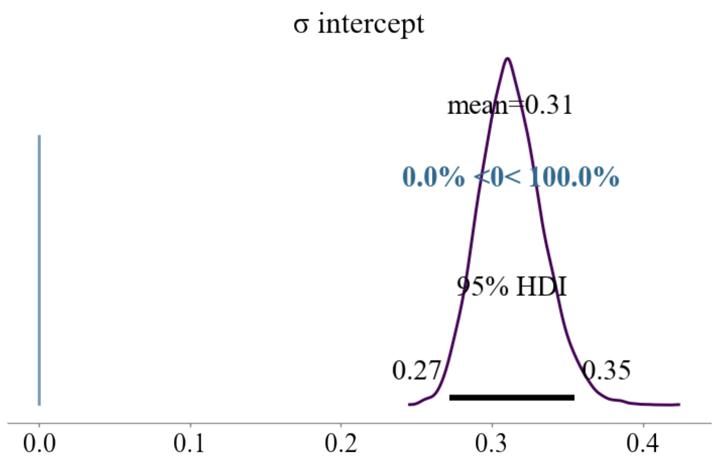

Figure A2: Posterior parameter distributions: notched impact strength; standard deviation of single linear model; 30CC.

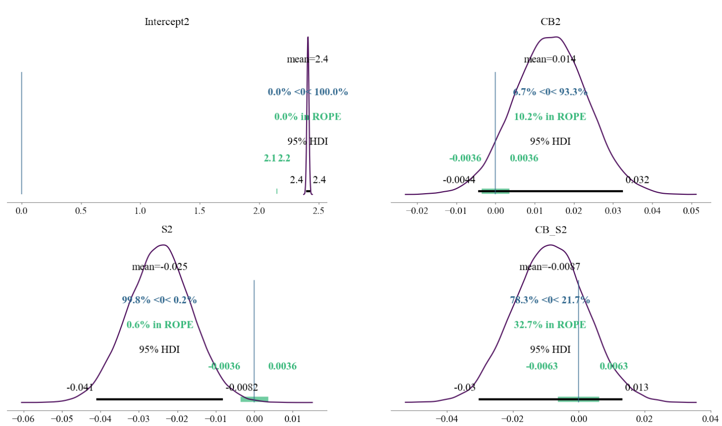

Figure A3: Posterior parameter distributions: notched impact strength; double linear model; high; 30CC.

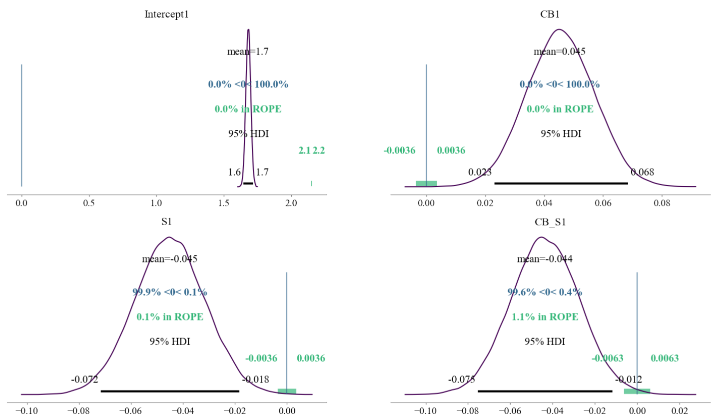

Figure A4: Posterior parameter distributions: notched impact strength; double linear model; low; 30CC.

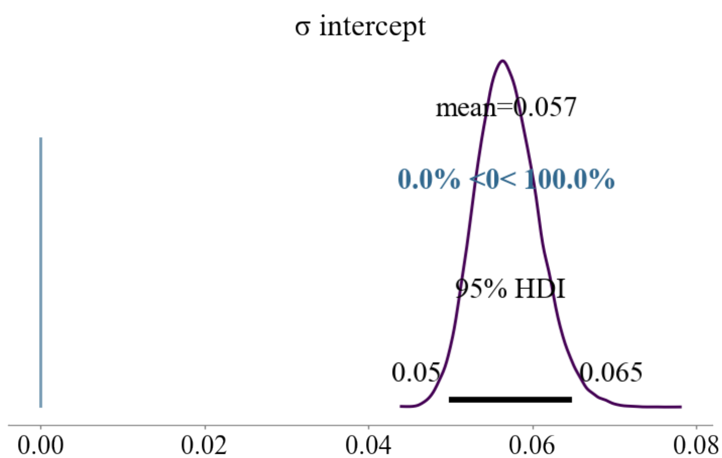

Figure A5: Posterior parameter distributions: notched impact strength; standard deviation of double linear model; 30CC.

A1.1.2. Effects of formulation

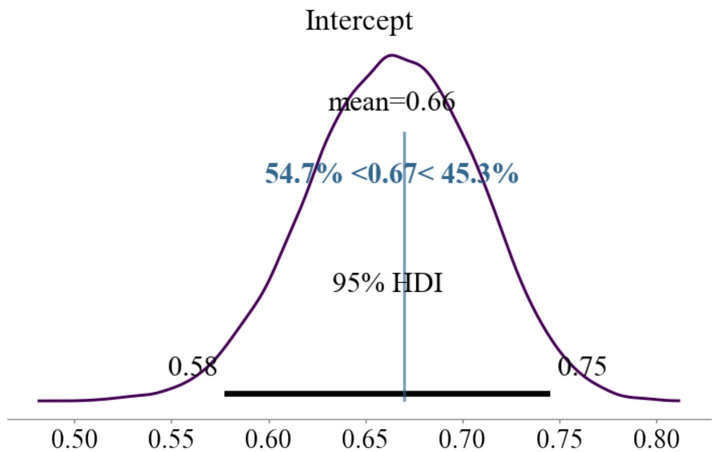

Figure A6: Posterior parameter distributions: notched impact strength; simple Bernoulli model; 30CC.

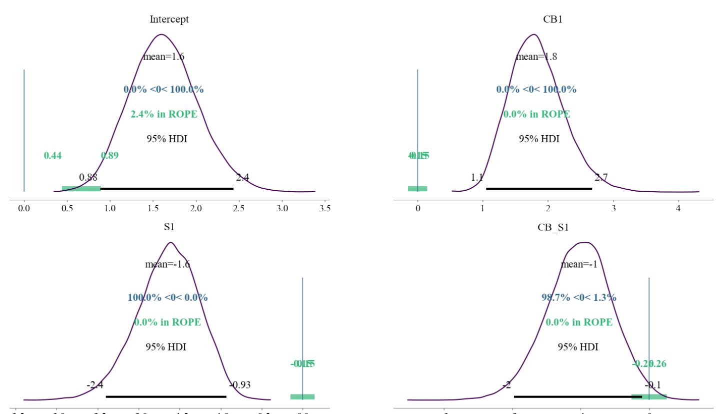

Figure A7: Posterior parameter distributions: notched impact strength; logistic model; 30CC.

A1.2. Goodness of fit

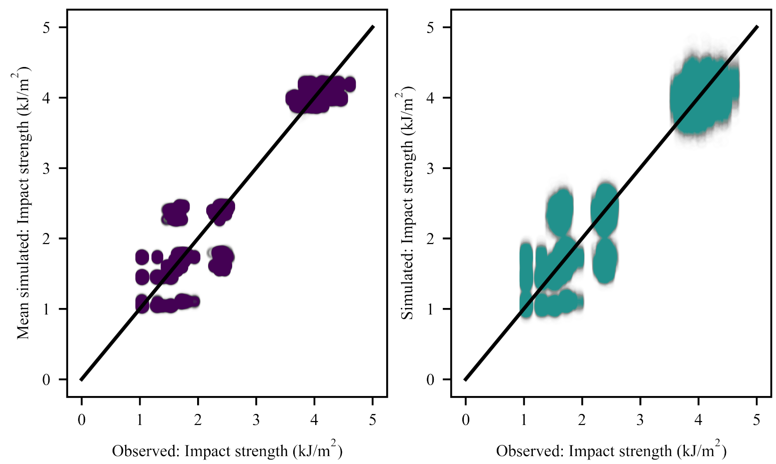

Figure A8: Goodness of fit: notched impact strength; full model, without (a) and with (b) noise.

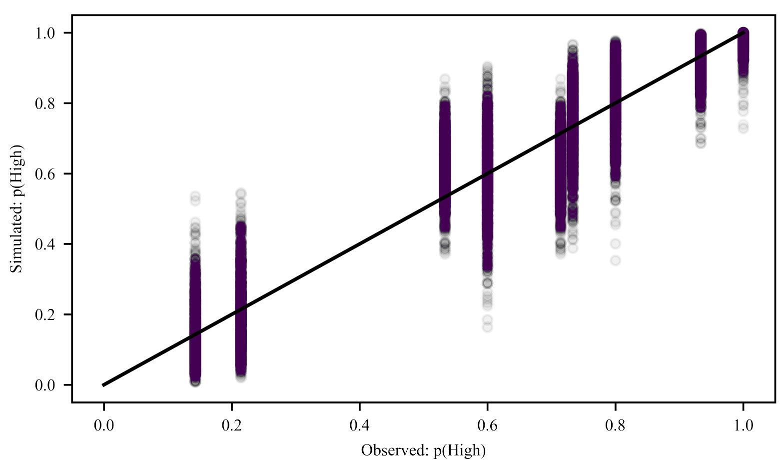

Figure A9: Goodness of fit: notched impact strength; logistic section of full model.

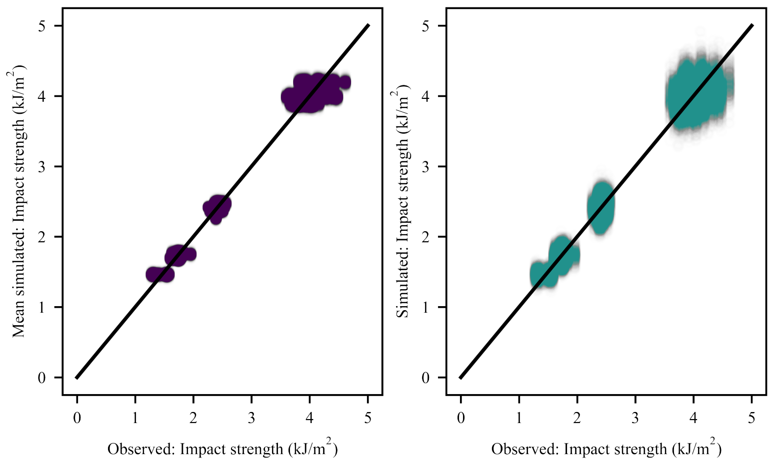

Figure A10: Goodness of fit: notched impact strength; higher linear model, without (a) and with (b) noise.

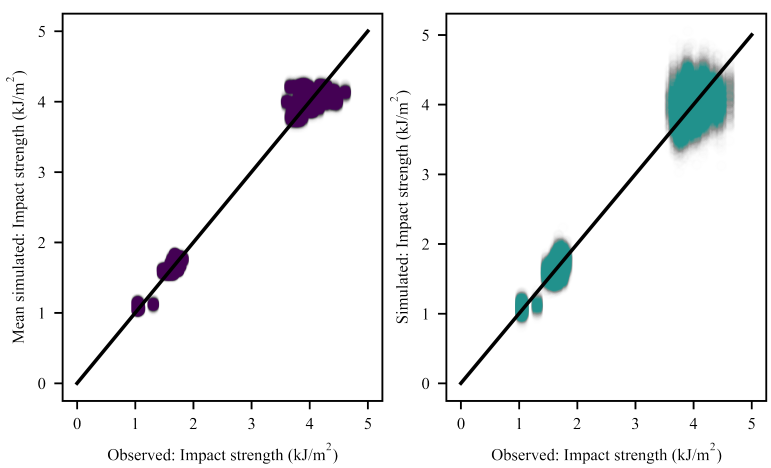

Figure A11: Goodness of fit: notched impact strength; lower linear model, without (a) and with (b) noise.

A1.3. Posterior parameter distributions

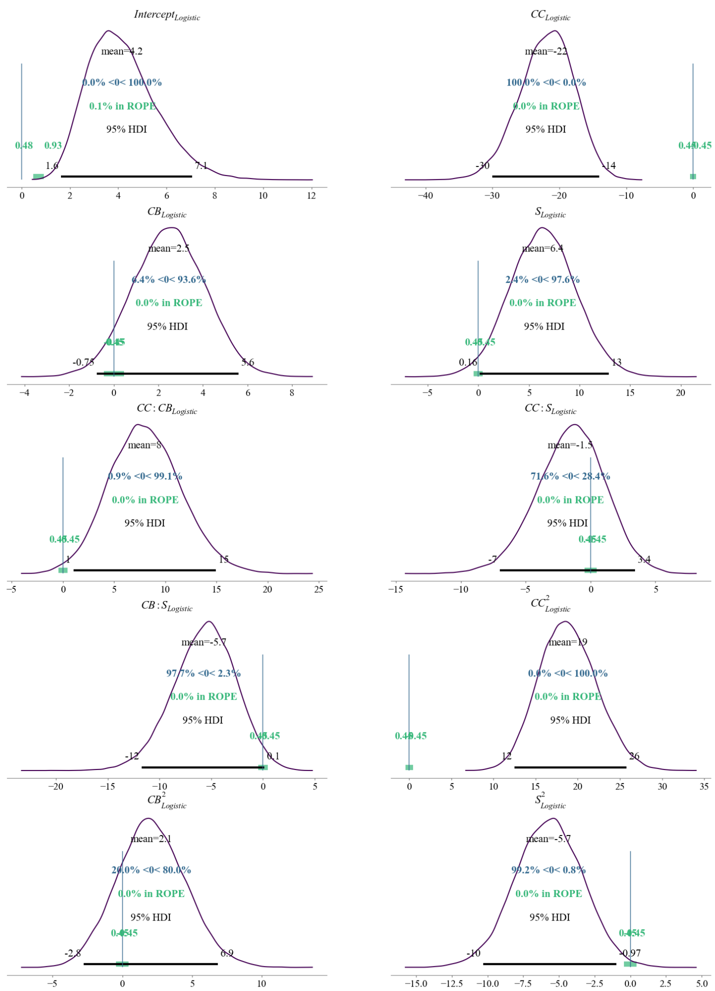

Figure A12: Posterior parameter distributions: notched impact strength; logistic section of full model.

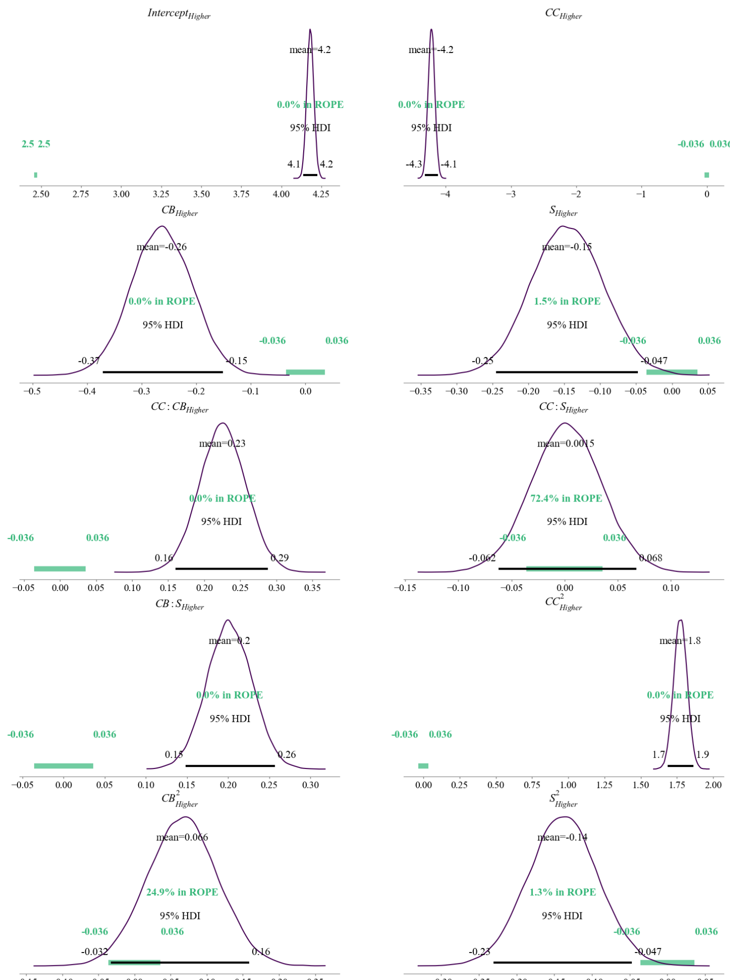

Figure A13: Posterior parameter distributions: notched impact strength; higher linear section of full model.

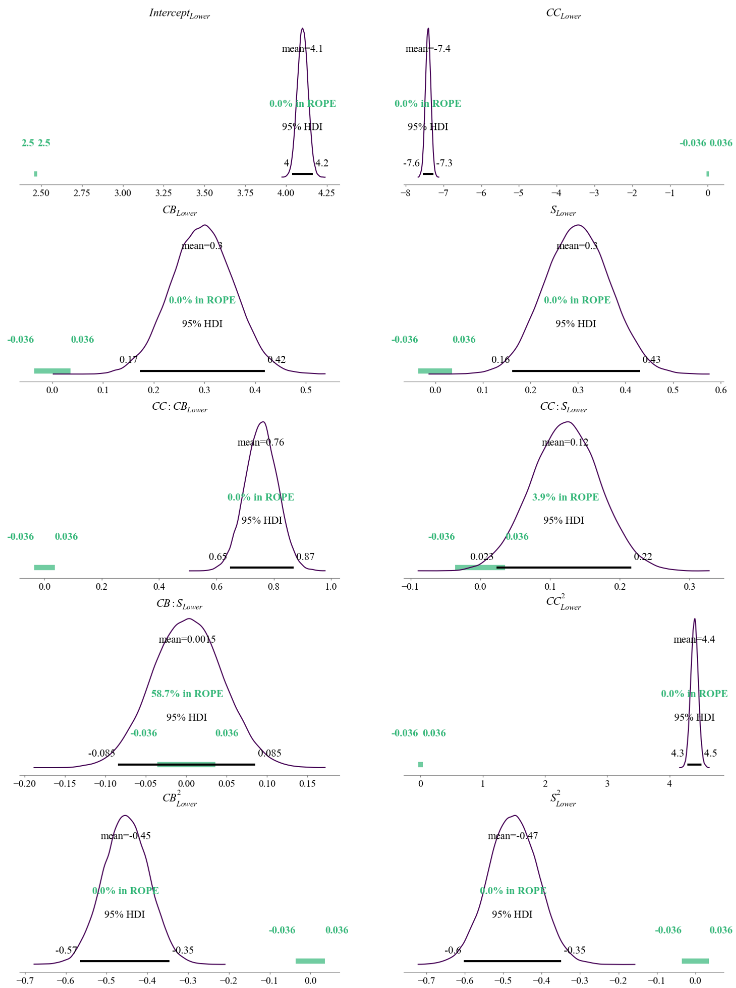

Figure A14: Posterior parameter distributions: notched impact strength; lower linear section of full model.

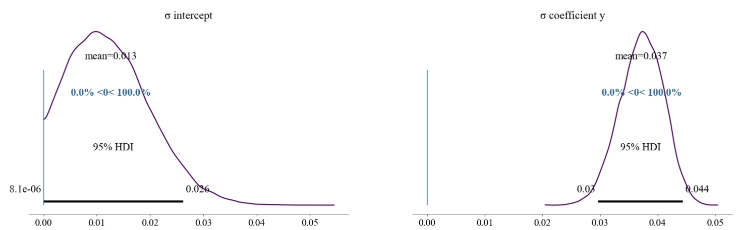

Figure A15: Posterior parameter distributions: notched impact strength; standard deviation of full model.

A1.4. Posterior probability of high-state failure: normalisation

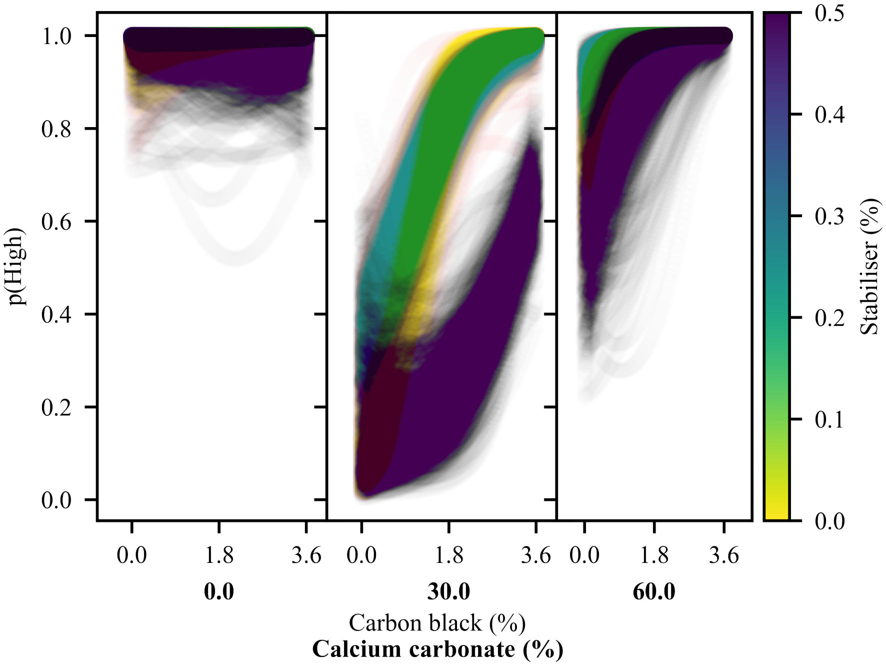

Figure A16: Plot of the posterior probability of high-state failure as function of the normalised formulational variables.

A2. Unnotched impact strength

A2.1. Goodness of fit

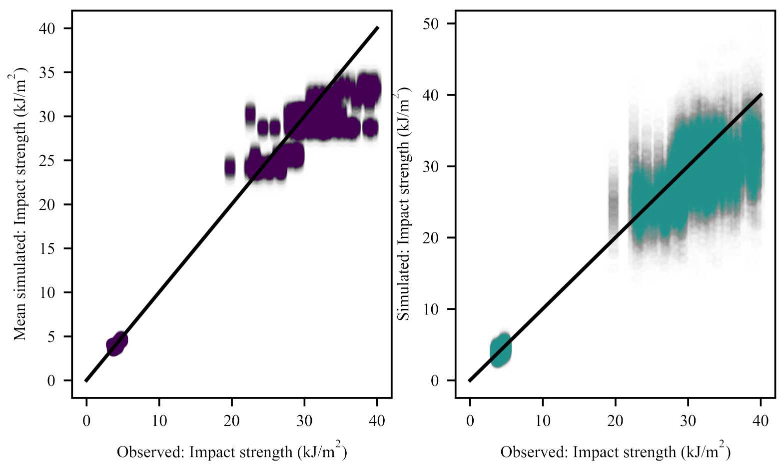

Figure A17: Goodness of fit: unnotched impact strength; linear model, without (a) and with (b) noise.

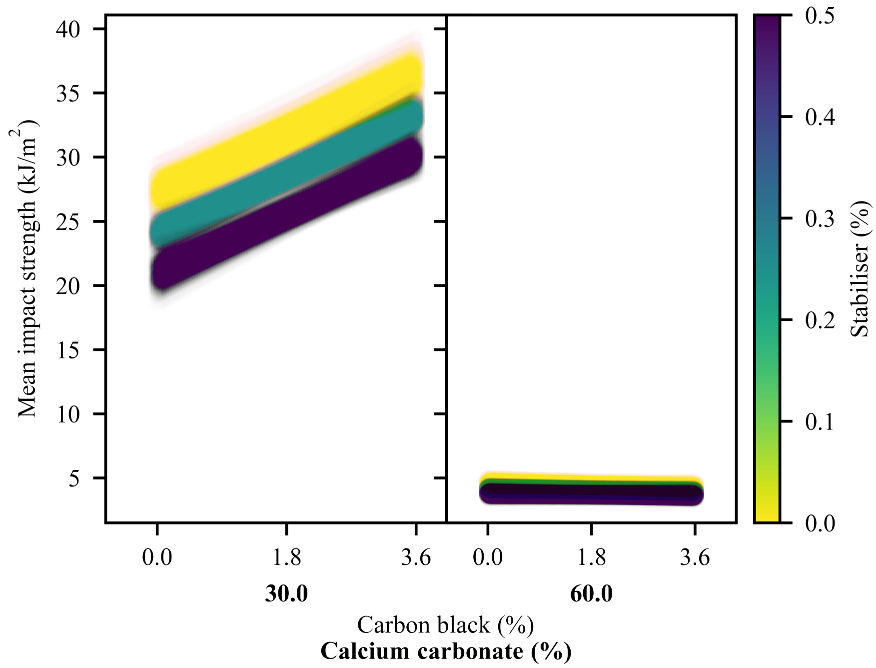

Figure A18: Posterior predictive fit: unnotched impact strength; linear model, mean.

A2.2. Posterior parameter distributions

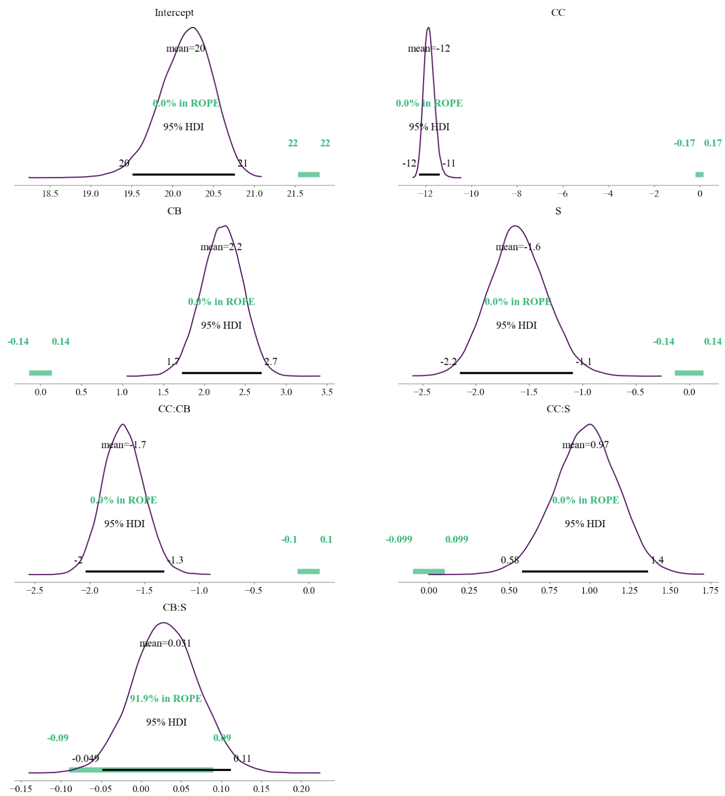

Figure A19: Posterior parameter distributions: unnotched impact strength; linear model.

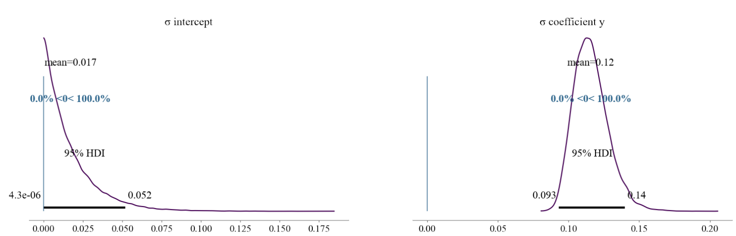

Figure A20: Posterior parameter distributions: unnotched impact strength; standard deviation of linear model.

A3. Crystallinity

A3.1. Goodness of fit

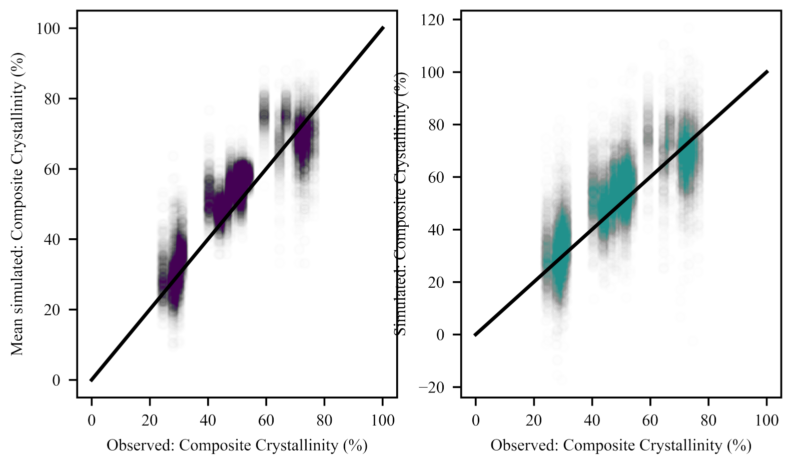

Figure A21: Goodness of fit: composite crystallinity; linear model, mean and with noise.

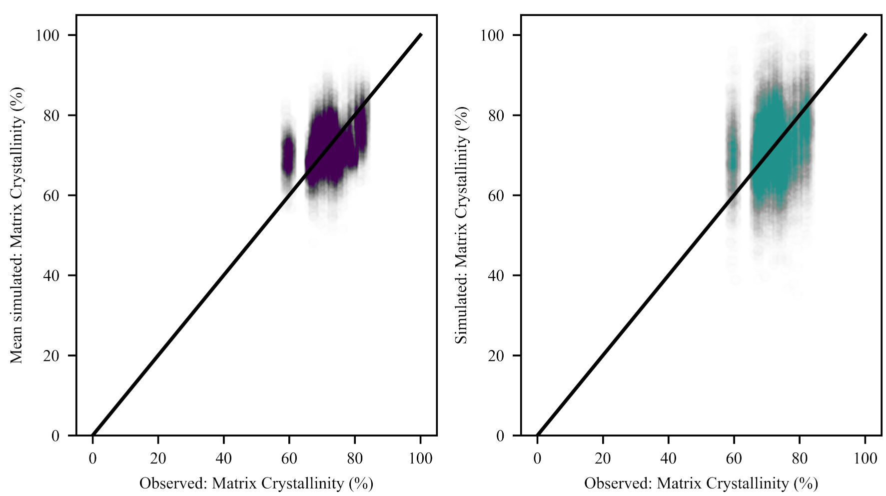

Figure A22: Goodness of fit: matrix crystallinity; linear model, mean and with noise.

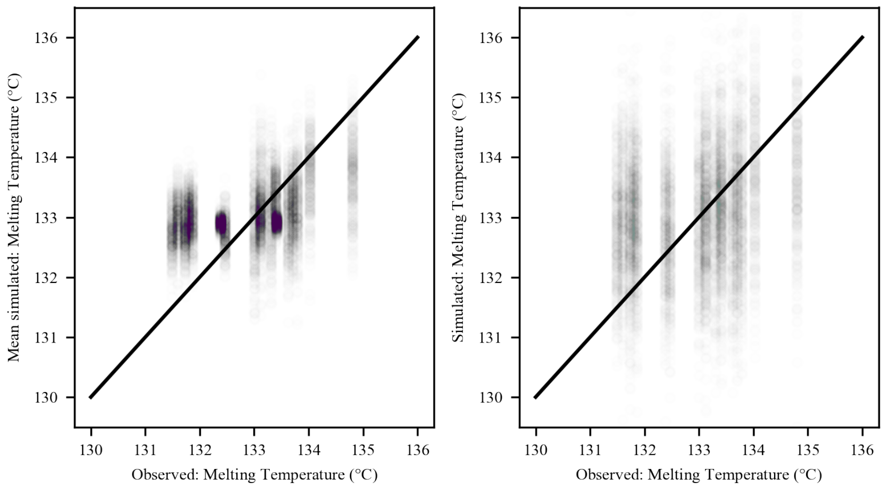

Figure A23: Goodness of fit: melting temperature; linear model, mean and with noise.

A3.2. Posterior parameter distributions

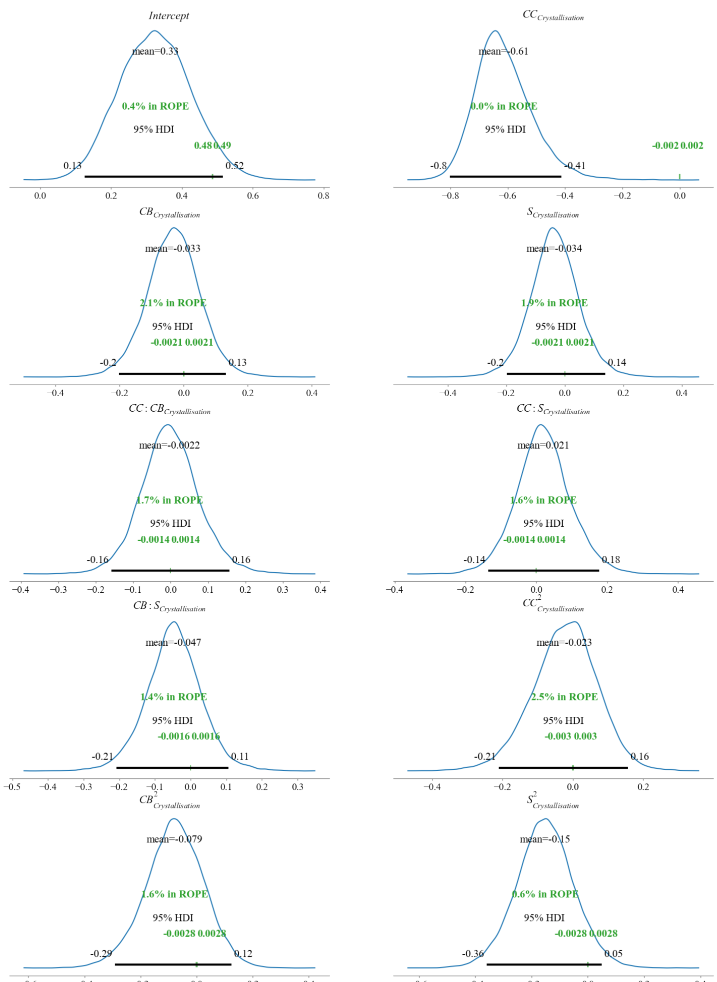

Figure A24: Posterior parameter distributions: composite crystallinity; linear model; melting.

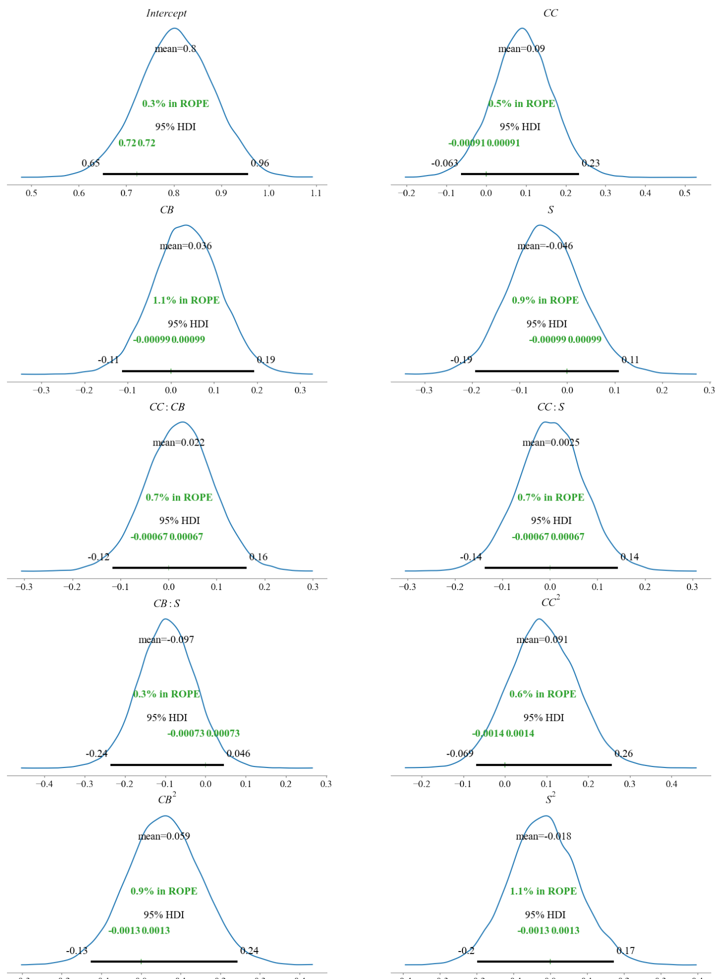

Figure A25: Posterior parameter distributions: composite crystallinity; linear model; crystallisation.

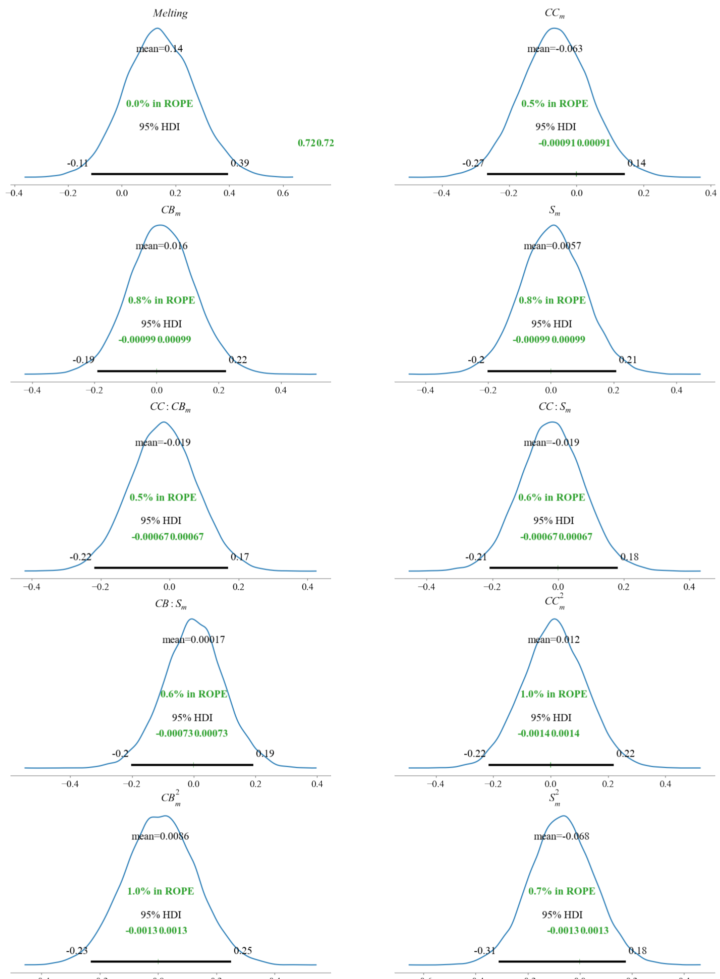

Figure A26: Posterior parameter distributions: composite crystallinity; linear model; difference between melting and crystallisation.

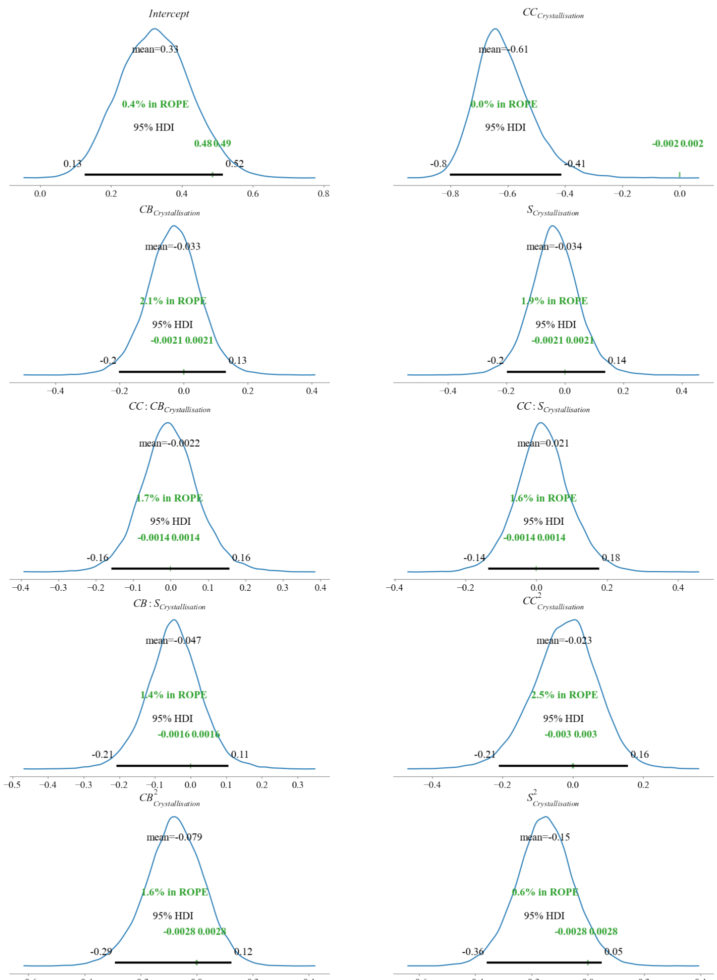

Figure A27: Posterior parameter distributions: melting temperature; linear model.