1 слайд

D: Our project is about composite resin cure kinetics. Composite materials are wildly used in aerospace. Every day 138 000 planes takes off with huge number of people onboard. On this figure you can see that materials have a significant role in the characteristics of the aircraft. We must to be confident that composite materials used in plane are cured well.

Y: Curing is the formation of bonds between the molecules of the resin. In aerospace used thermoset resins. Thermoset means that you can heat resin and it will come from fluent to solid, like omelet. One difference – resin produce heat during curing.

D: To measure this heat, people use differential scanning calorimeter (DSC). It heats resin with constant temperature ramp and measure difference between temperature of sell with resin and empty one. So in this project we used data from that DSC measurements. Our task for this project was to try modern ways to simulate composite curing and afford new one based on ML.

2 слайд

Y: First of all, we download and plot data for one measurement. Here you can see plots of DSC signal on time and on temperature. They look similar, because DSC heat resin with constant temperature ramp.

The resin cure degree (alpha) calculates as ratio of current exploded heat to total heat for used resin. To calculate it we need to separate curing peak from all data

3 слайд

D: Here we can see find\_peak function where we calculate peak starting points, widths and height. To perform this task we use scipy modules. The result can be seen on the plots.

Y: Here we can see function, which normalize our peak. And now we can integrate it to get total exploded heat. Now we can construct cure - alpha degree in time

D: We integrate normalized peak data using simpson method and then add partial sum divided by total spent energy. Thus, we receive array of values of alpha.

Y: Our task was do develop model, witch will fit data better than models used on facilities. To calculate its error, we shall first of all build it. On slide you can see kinetics equation based on Arhenius chemical reaction model. It allows to calc next cure degee on each time. On input it get resin constants and temperature.

D: in order to solve the equation we need to take a logarithm and perform linear regression on dalpha by dt, using alpha as a feature. Linear regression will give us coefficients which specify the resin.

Y: To fit liner regression we need one more iteration for data preprocessing. Here you can see dataframe construction based on measurement

D: On this slide you can see the linear regression itself. Firstly, we create our features and targets, using data, processed step before and then fit it. After that we can easily compute equation coefficients.

Y: Function, witch calculate alpha on d\_alpha per d\_time. Here plotted experimental peak and model based peak. You see that this model doesn’t fit our data great. On right plot constructed cure degree for experimental data and model based. Plots are good, but lets look at numbers. R2 is 0.99. Let’s try and another approach without Arrhenius equation.

D: First of all, lets select features and targets. We choose alpha and temperature a features and dalpha per dtime as a target. Then we want to take a look at how our data is distributed. It doesn’t seem that linear regression will fit our data really good, but let start with the simplest model.

Y: Data is devided to test and train. So here you can see linear regression fit and errors calculation. You see, that linear regression doesn’t fit our data well. At right plot orange – real experimental alpha, blue is predicted resin behavior.

D: Well, our second thought was to use polynomial features in order to improve situation a little bit. And performance is far-far more fabulous. And the plots illustrate it.

Y: We want to be honest with you and potential customers. So we decided to check error with cross validation. And ooops… R2 becomes worse.

D: Lets compare errors of different models more thoroughly. First, we will take a glance on MSE errors. Obviously, linear regression with polynomial features error is the smallest. But its cross validated error is the same order as linear regression error.

D: Probably, more descriptive will be r2 plots. Here we can see that linear regression without polynomial features cannot perform as good as polynomial model.

Y: Lets go further and try to use grid search, which will find best parameters for polynomial model. Choose before polynomial degree wasn’t optimal. After that, we repeated these steps for more complicated dataset. This dataset holds DSC measurements for one resin on different heating rates. It’s Important to fit model on multiple measurements because with it we can better calculate curing rate on different heating ramps.

D: Some more pandas… We performed the same steps for all our datasets and then concatenated them.

We refitted our model using parameters obtained via GridSearch and the error is acceptable. Unfortunately, severe time constraints didn’t let us to perform proper comparative analysis of all models. But it is our plans for further research.

Y: Let’s make little sum up. We processed DSC dataset of one resin cure measurement and implemented classical method for calculating resin cure degree. After that, we used different types of regressions to refine that classical method.