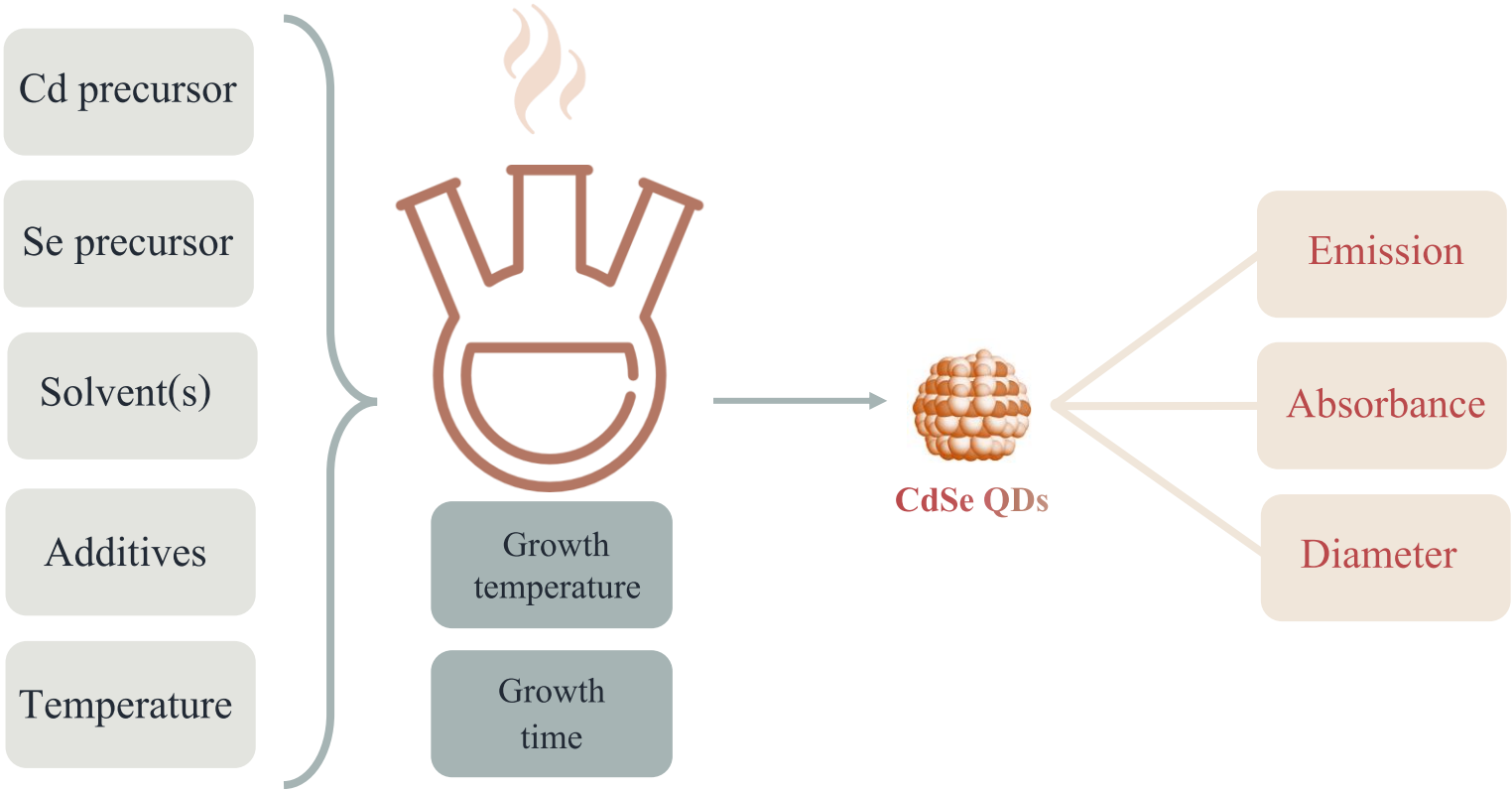
Hot Pots for Good Dots

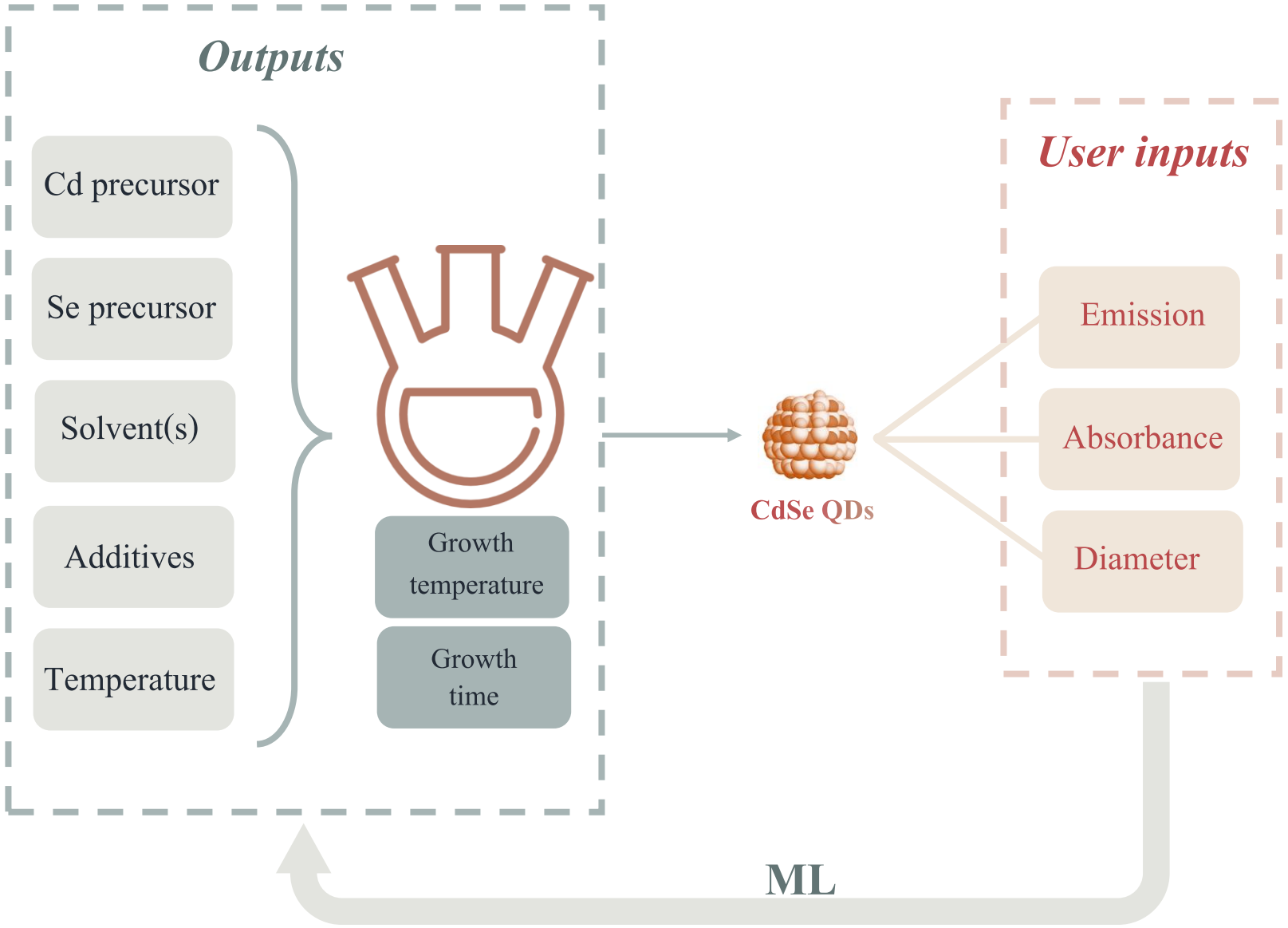
Typical synthesis of CdSe quantum dots (QDs)



User case 1

Story:

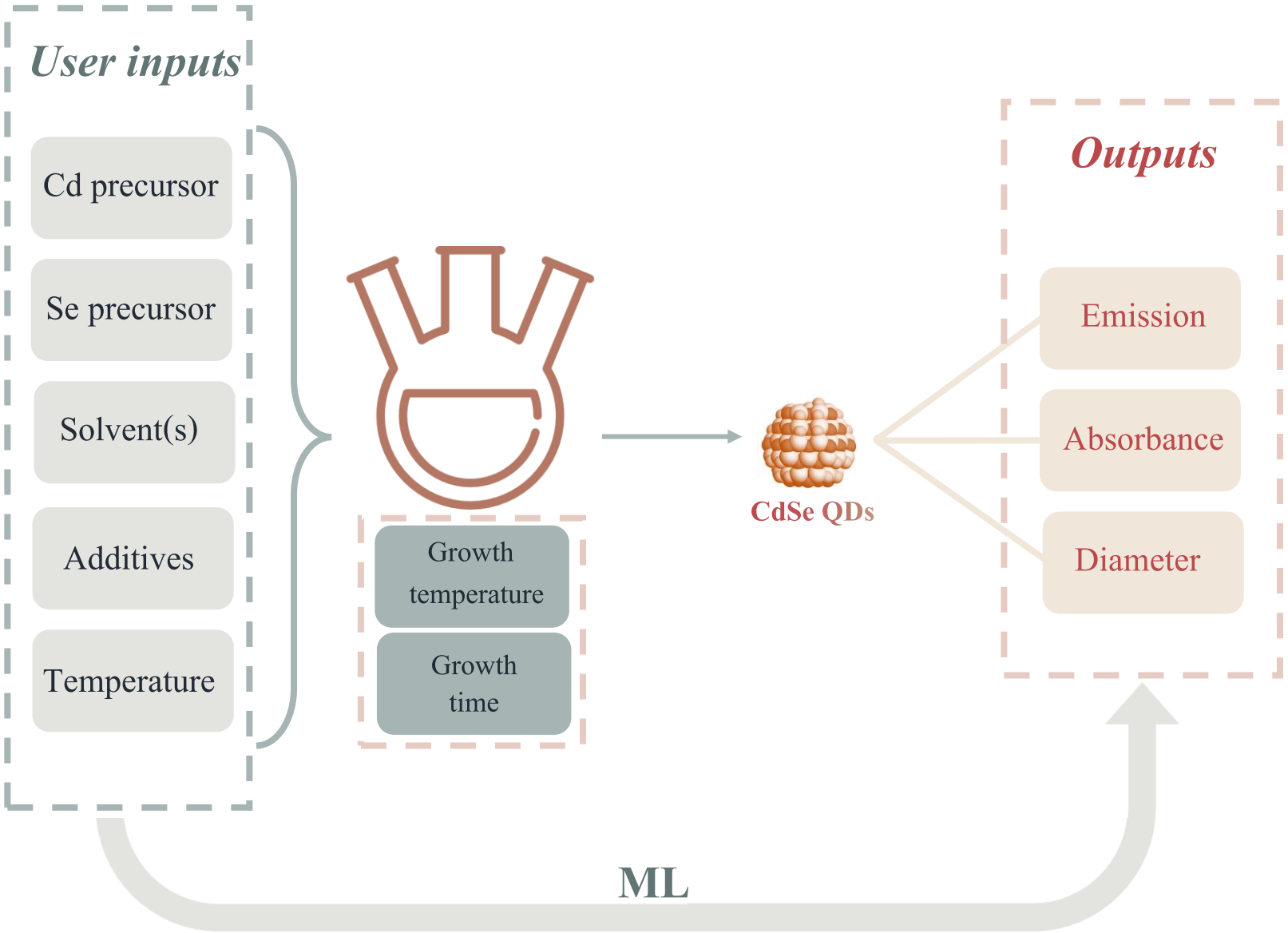
Alex is a chemistry udergrad student, and he wants to synthesize CdSe quantum dots. The material Alex wants is very specific: CdSe quantum dots that emit at 580 nm and have a diameter around 3.7 nm. However, he is new to this field and there are so many procedures in the literature. The procedures are not even consistent. Alex doesn't know which procedure to follow, and he doesn't have time to read all of the papers. Alex is confused.



User case 2

Story:

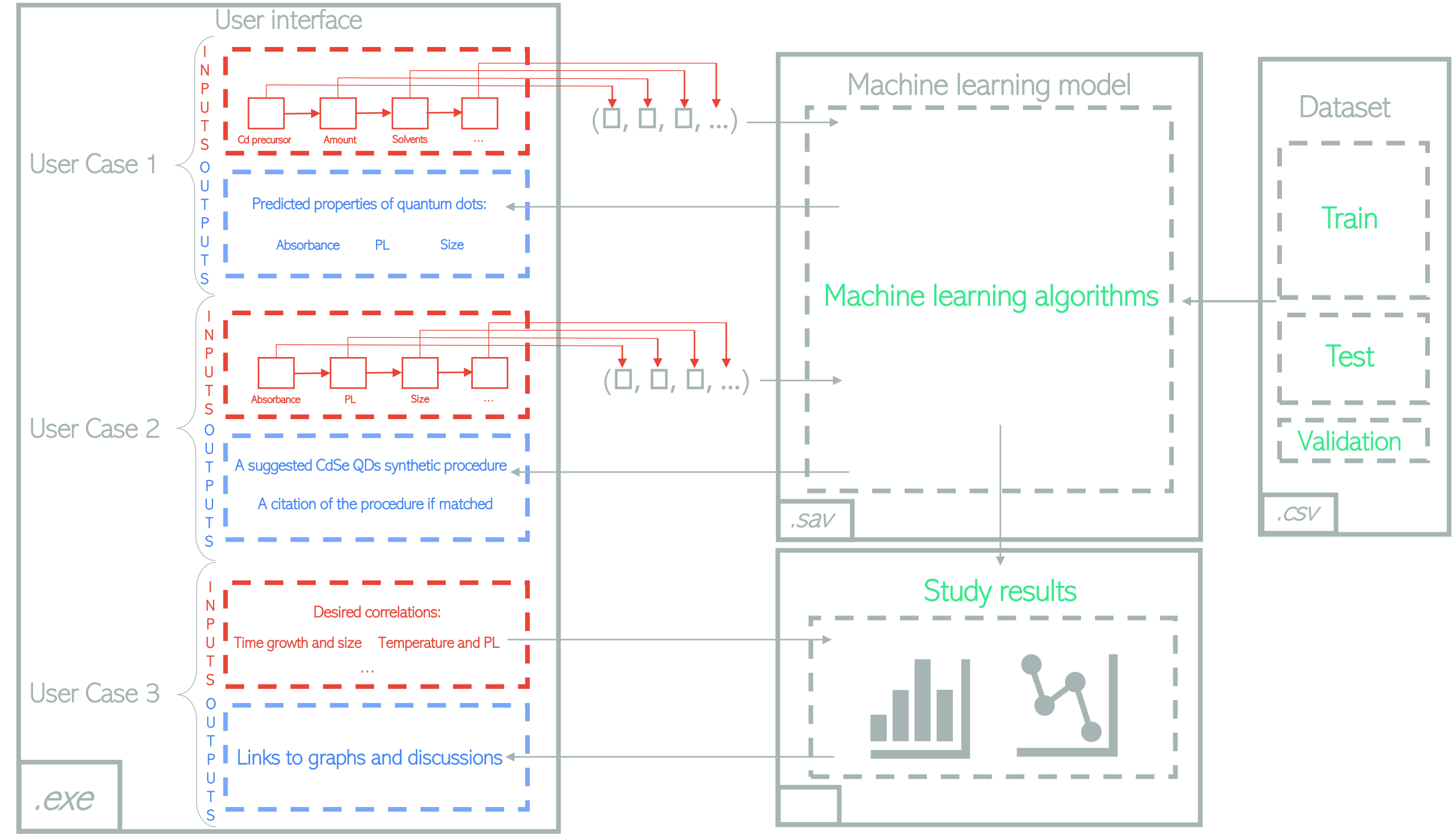
Clay is a chemistry grad student who has some experience with syntheses of nanoparticles. He has just run one experiment to synthesize CdSe quantum dots. The next thing in Clay's agenda is to run a dozen more of the experiment with modified conditions. He wants to adjust the temperature and the solvents of the reaction to see if the outcomes are different. But Clay can only come to the lab twice a week due to Covid. Clay knows in the group meeting on Friday, his PI will be mad if he doesn't have a prediction of how changing the conditions would affect the syntheses. Clay is frustrated.



User case 3

Story:

Zach is a chemistry professor who studies syntheses and properties of colloidal nanocrystals. He knows that, despite the substantial improvement over the past decades, all synthetic techniques are Edisonian (trial and error)-based QD synthesis. Zach thinks if he looks at many procedures, considers synthetic conditions, the outcomes, and finds the correlations between parameters, he may figure a systematic way to synthesize QDs. Zach is curious.


User interface
User Case 1
INPUTS
Cd precursor
Amount
Solvents
...
OUTPUTS
Predicted properties of quantum dots:
Absorbance
PL
Size
User Case 2
INPUTS
Absorbance
PL
Size
...
OUTPUTS
A suggested CdSe QDs synthetic procedure
A citation of the procedure if matched
User Case 3
INPUTS
Desired correlations:
Time growth and size
Temperature and PL
...
OUTPUTS
Links to graphs and discussions
.exe
(□, □, □, ...)
(□, □, □, ...)
Machine learning model
Machine learning algorithms
.sav
Dataset
Train
Test
Validation
.csv
Study results