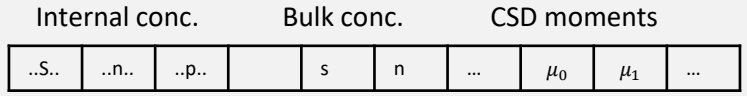
Initialize the system:

- Biocatalyst loading → enzyme conc. in carrier
- Total Enzyme mass → total number of carriers
- Reactor volume
- Initial conc.
- Initial pH

Using the initial conc. define the system's state vector $\vec{u}$ for the discritized spatial domain with three parts:

1- Internal conc. in the carrier
2- Bulk phase conc.
3- Crystal moments (nonzero if seeded)



Explicitly solve the set of ordinary differential equations (ODEs) . At each timestep:

Reaction-diffusion module:

1- If pH is fixed, calculate the required titrant (Na^+), update its bulk and interface conc. and reactor volume
2- Based on the current state, calculate the local pH using equilibrium constants and electroneutrality
3- Based on the local pH, calculate the amount of each species in charged and neutral state at each node
4- Using equation (2-3) calculate the flex of each species
5- Using equation (1) find the consumption/production rate of each species due to reaction
6- Calculate the overall rate of change due to reaction and diffusion for each species at each internal node
7- Calculate the rate of change in the bulk using mass conservation at the interface

Crystallization module:

1- Calculate the solubility based on current bulk pH and solution's ionic strength
2- Calculate the supersaturation of the product
3- If supersaturation is > 1:
    i. Calculate the primary nucleation rate
  If supersaturation is > 1 and moment of CSD != 0:
    i. Calculate the secondary nucleation rate
    ii. Calculate the growth rate
4- Calculate the overall rate of change of CSD moments using B and G
5- Update the rate of change of bulk and interface conc. for the crystallizing agent