Modeling of geochemical processes

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An Introduction

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Reality and subjective vision
Observation and experiment
Model

Previous concept

- ***model*** – a real object in the lesser scale;
  an attempt to imitate original
- applications in engineering:
  behavior of the model was extrapolated to the behavior of the ***original object*** (a presumption that both behavior will be similar)
- Risk that the model behavior is different
  Similarity Theory, Dimensional Analysis (dimensionless variables, size analysis)

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Modern concept

- ***model*** is imaginary – it reflects the physical idea

  Model replaces the physical reality with an identical mathematical description.

- ***Models*** describe the behavior of physical system in the given range of variables and precession. Model is not identical with real object.

- We periodically find that model is not valid for certain range of variables or that it is not precise enough! Based on these facts, ***new model*** is derived – model more precise (often more complicated a less visual).

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Actual **physical principles** (theories, theorems, hypothesis) "satisfactory" ***describe*** the behavior of natural systems; at least, in the range of the condition at which they were verified!

Example: gas equation **pV = nRT**

The model introduces ***ideal gas.***

Any real gas does not respect this equation (model).

In general, however, the model (equation) is frequently used!

If its preciseness is not satisfactory, the more precise model based on the more complicated picture (van derWaals model).

Sometimes a reality is described without any picture, based on mathematical description (phenomenological approach).

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Model development

A. Formulation of a physical model

Formulation of a vision, simple as possible; validated by an experiment

The tools

- *balances* (mass balances, energy balances, charge balances...)
- *equilibrium equations* /heat -, chemical -, phase- equilibrium/
- *rate equations* /mass fluxes/

Tools are often combined!

Simplification

- little influences are neglected (activity coefficients, deviations from ideal behavior, deviations from constant values...)

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- a vicinity is assumed to be constant (temperature, pressure…)
- system is considered to by homogenous (stirring, diffusion...),
- continuous system is replaced by discontinuous one
- variables are presumed to be constant (surface area, pH....)
- dependences are understood as linear (linearization…)
- random changes of some variables are neglected (stochastic model is replaced by deterministic model)

After reaching basic behavior and properties, model can be improved (model complicates)!

B. Mathematical solution

Mathematical solution of the model results into the solving of systems of differential equations – linear or non-linear (numeric methods, computers)