Dynamic Programming Using the SimuSage Component Library and its Application to the Simulation of the Cement Clinker Burning Process

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Abstract

In mathematics and computer science, dynamic programming is a method of solving problems exhibiting the properties of overlapping sub problems and optimal substructure (i.e. optimal solutions of sub problems can be used to find the optimal solution of the overall problem). In general a problem with optimal substructure can be solved using a three-step process:

- Break the problem into smaller sub problems
- Solve these problems by using this three-step process recursively
- Use these optimal solutions to construct an optimal solution for the original problem

The sub problems themselves are solved by recursively dividing them into sub problems until some simple case is reached that is solvable in constant time.

For the thermodynamic simulation of a complex process dynamic programming can be used to break down the overall problem into recurrent substructures recursively until simple structures are obtained. Using the SimuSage component library these structures are the SimuSage components. Combining these unit operations more complex units (types and classes) can be constructed. By further giving these units properties (e.g. temperature, heat transfer coefficients) and methods (e.g. calculate heat transfer, calculate phase amounts in equilibrium according to reaction kinetics) they can be easily accessed, processed and further combined. Hence a complex process can be described by connecting predefined substructures. After setting the necessary parameters (properties) these substructures can be calculated whereby necessary properties are passed on to internal substructures and then calculated by calculating their internal substructures and so on. The big advantage of this procedure is the flexibility to changing model layouts for complex processes.

In the cement clinker burning process the recirculation of volatiles (especially alkali salts) plays an important role and contributes to wear of refractories in the kiln. Alkali salts are accumulated by an evaporation/condensation process interacting between the kiln atmosphere and the kiln feed, and are infiltrated into the bricks by condensation from the vapor phase. In many cases it is desirable to predict the loading of refractories by alkali salts in dependence of varying process parameters. Especially changes of fuel are of great importance nowadays. Introduction of petrol coke may significantly raise the sulfur input; polymers may contain chlorine. A prediction of the volatile recirculation caused by changes of process parameters may e.g. help to optimize refractory selection and estimate the impact of process technology on wear.

In order to fulfill this goal calculation of volatile recirculation is performed by means of process simulation using the dynamic programming approach described above. Substructures are defined to model elementary process steps (e.g. preheater stage, calciner). The rotary kiln itself is discretised into several sections, each of them represented by a substructure. These substructures establish balances governing mass and heat transfer, and enable the calculation of chemical equilibrium. The total of these balances sets up a nonlinear system of simultaneous equations which is solved by a numerical iteration procedure. As a result, the chemical composition of internal solid and gaseous mass fluxes is available. In combination with a thermal simulation of the kiln lining the infiltration of alkali salts into the refractory can be calculated additionally.