3-D Computer Simulation of Electron Beam Cleaning Processes

A.S.Petrusev, B.V.Potapkin, E.V.Shulakova, A.A.Fridman

Kurchatov Institute of Atomic Energy
Kurchatov Square, 123182, Moscow Russia

The electron beam processes attract a great interest via such applications as a treatment of different chemical gas impurities: SOx, NOx, halocarbons, mercapthanes and so on. Several zero dimensional computers code were developed for the modeling and optimization of Electron Beam Process. These codes (the most detail and precise was developed in KFK, Germany [1]) were in a good agreement with the experimental results and permits to define the chemical mechanism of the DeSO2/DeNOx EB process. Nevertheless the process efficiency, as it was shown in the result of recent research, can strongly depends on dose and dose rate distributions in process vessel, reactor geometry and hydrodynamic conditions. Heterogeneous reactions on the surface and inside of aerosols particles produced during EB process can also have dramatic effect on the removal efficiency. Therefore, 3-dimensional numerical model of the chemical processes initiated by electron beam for the real reactor geometry, dose rate distribution in time and space and gas velocity distribution has been developed.

In addition to gas phase reactions the following physical and chemical effect were taking into account: three dimensional hydrodynamics (the process kinetics can be calculated for the definite gas velocity distribution in the reactor); dose rate distribution in process vessel both for the continuous and pulse electron beam; molecular

and turbulence diffusion mass transfer the heterogeneous oxidation and reductions including reactions in the droplets on the surface of aerosol particles reactions, The model includes the chemical kinetics and 3-dimensional hydrodynamical continuity equations to take into account the nonuniform chemical processes.

For numerical solution of this equations the droplet-step method has been used. At first substep the stiff system of chemical kinetics equations have been solved. At second, third and fourth substeps the diffusion equation have been solved at the X-, Y- and Z- direction respectively.

The solution of chemical kinetics equations have been obtained via the implicit multistep Gear-Nordsieck method with automatic control of internal time step. To solve the diffusion equation with relatively large flow item the implicit method with nonuniform "progonka" have been used, which provide stability of the algorithm at the large time-step values.

The calculation via droplet-step method some specific difficulties includes [2]. Generally, there are boundary condition (at the diffusion calculation), choice of time step value and step of the grid.

The boundary equations in our case are:

$$n_i = n_{i0} \qquad z=0 \tag{1}$$

$$dn_i/dz = 0; \quad z=z_{out} \tag{2}$$

$$dn_i/dG = 0; \quad dQ \tag{3}$$

Where n_i- concentration of i^{th} component, n_{i0} - initial concentration at the input cross-section, z_{out} - output cross-section, dQ - side surface. The finite-difference

approximation of first and second equations have no difficulties, but third equation in case of non-rectangular geometry includes X- and Y- derivatives simultaneously. It lead to instability of calculation scheme due to Curant [2] criterion, because the scheme becomes explicit in boundary nodes. To illuminate this difficult my be used sequence of small time steps at the diffusion calculation or adaptive grid, which provides coordinate axis, orthogonal to the boundary surface. The large difficulties of second way lead us to using the first way, in which time consumption of diffusion calculation is still less then chemical one.

The time step choosing includes following aspects: calculation precision and stability of numerical scheme.

$$dn \sim o(Dn_{chim} \pm Dn_{diff}) \quad (4)$$

where Dn_{chim} Dn_{diff} changing of concentration at single step in chemical and diffusion calculation respectively, dn - calculation error. Some initial steps may be rather large, then steps value should be decrease. In case of time-dependent EB distribution, the time step should be less then characteristic time of EB swapping.

The stiff chemical system of equations contains, generally, two time scales, T and t, where t < T. t scale is proper to quick, "stiff" components. As a rule, there are ions and short-life radicals. T scale connects with secondary long-life products. With excluding the EB swapping time, the success of calculation requires three conditions:

$$t \ll h^2/D \quad (5)$$

$$t_{step} \ll T \quad (6)$$

$$t_{step} \sim h^2/D \quad (7)$$

Where t_{step} - time step value, h - step of the grid, D - diffusion coefficient. The conditions (6),(7) connects with (4). Condition (5) is due to avoid the disturbance of the stiff components and supply stability of calculation scheme. To satisfy conditions (5)-(7) it is necessary, that

$$t \ll T \qquad (8)$$

which, as a rule, is true in stiff chemical system. But there are kinetic schemes, which contain continuous set of chemical time scales rather than distinguish difference (8). If it is the case, there are difficulties of time step choice may by arisen, which led to instability of calculation.

Practically, t time scale is obtained from the Gear procedure in each node, and is the minimum of internal time step respectively. Under there data obtained, it is no difficult to automatic control of the global time step value with the aid of criterions (5)-(7). If the step of the grid h gets no opportunity to satisfy (6) and (7) simultaneously, it leads to stopping the calculation, and changing of the grid.

This model is used for numeric modeling of the NOx elimination EB-process. The removing degree have been obtained at different values of the space dose distribution, electron energy and dose power both for single and double-hold electron irradiation. It was shown in particular that heterogeneous reaction during the stages play more important role with respect to effects related with non-uniform dose rate distribution.

REFERENCE:

1.Matzung H. Chemical kinetics of flue gas cleaning by electron beam.
Kernforschungzentrum, Karlsruhe, KFK 4494, 1989.
2.Samarsky A.A. Theory of difference scheme. (in Russian)
M. Moscow, 1977.