Neutralization Tank

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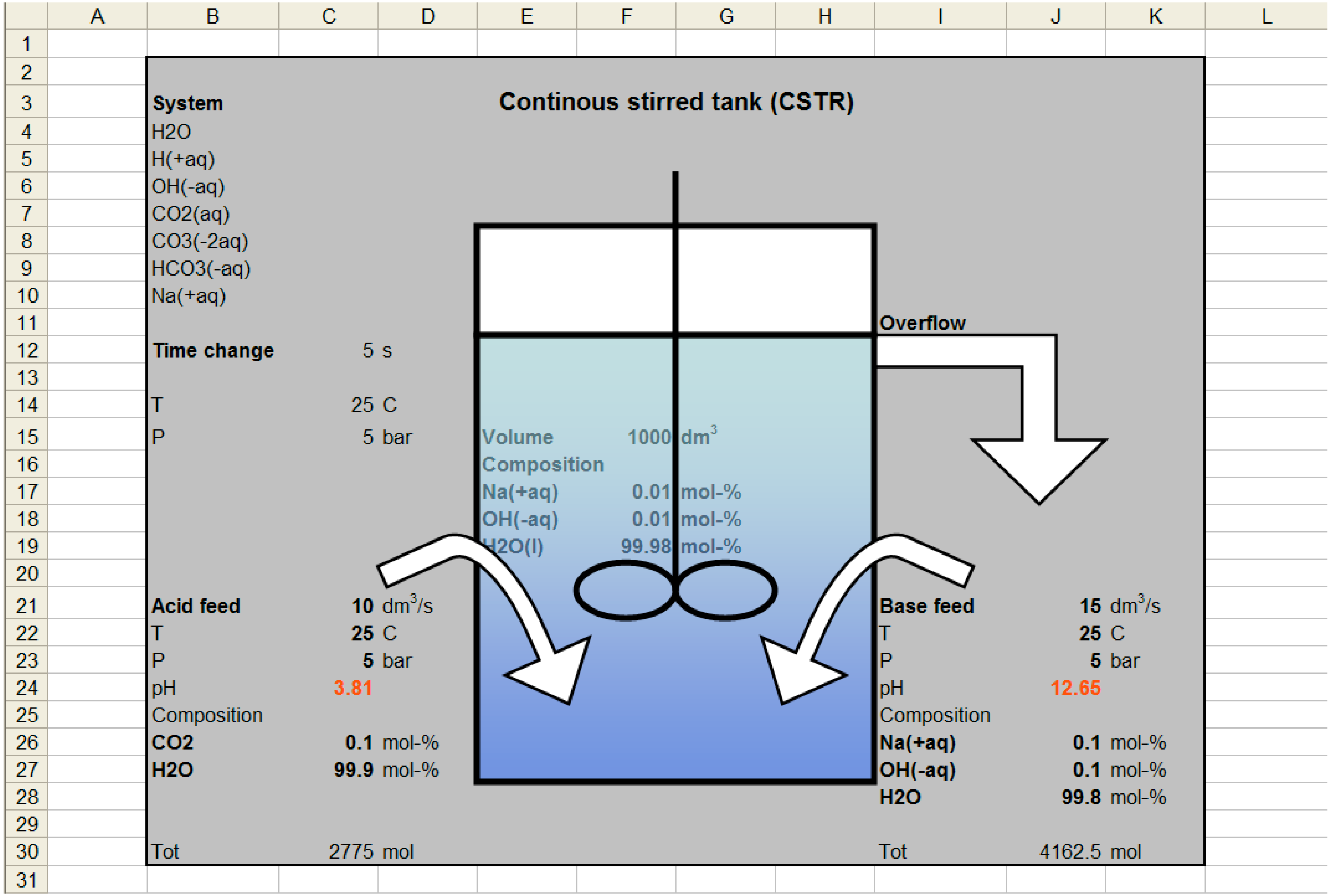
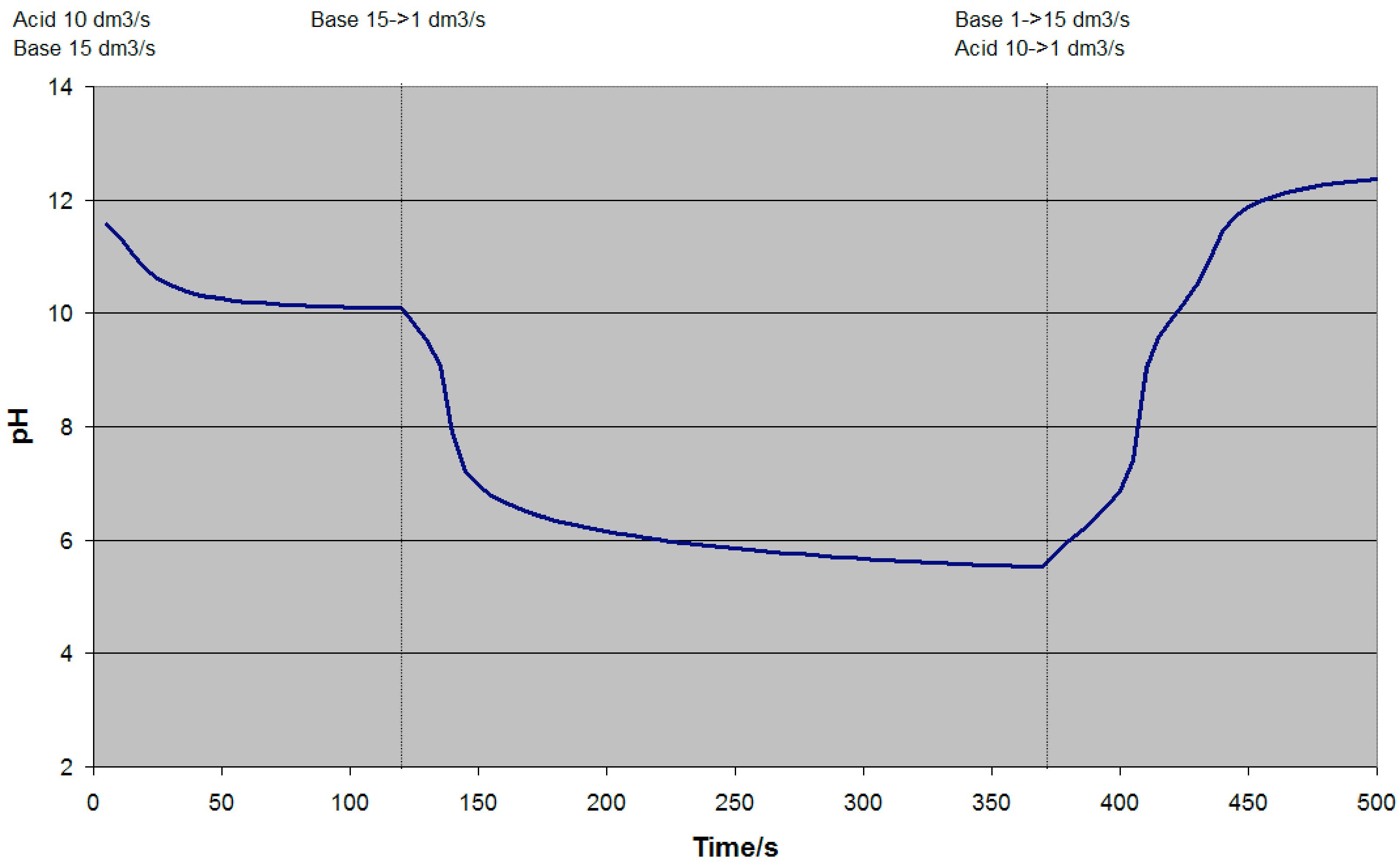
ChemSheet Model



Assumes instanteneous mixing (no delay) = not accurate

ChemSheet Results

Ideal mixing (1000 dm3, start pH 11.56 (NaOH+H2O)), pH as function of time



CFD Model

The objective of this work was to study the possibility of calculating the reactive mixing process by joining the two commercial programs, Fluent and ChemApp. In Fluent, chemical reaction rates can be modelled based on finite rate. The species transport can be modelled with or without chemical reactions. In the study, the chemical reactions were related to equilibrium calculation results from ChemApp. In ChemApp, the calculation of chemical balance is based on the minimization of Gibbs energy.

In the study, the joining of Fluent and ChemApp calculations was tested by the case of neutralization process where solution reactions were assumed fast. In the process, aqueous solution containing dissolved natrium hydroxide in a stirred mixing tank was neutralized by adding dissolved carbon dioxide into it.

The effect of micromixing by the turbulence was studied by the model of eddy dissipation concept EDC. In the EDC model, the reactions are assumed to take place only in a part of the computational cell where the reactants have been mixed due to the turbulence.

Geometry&Grid

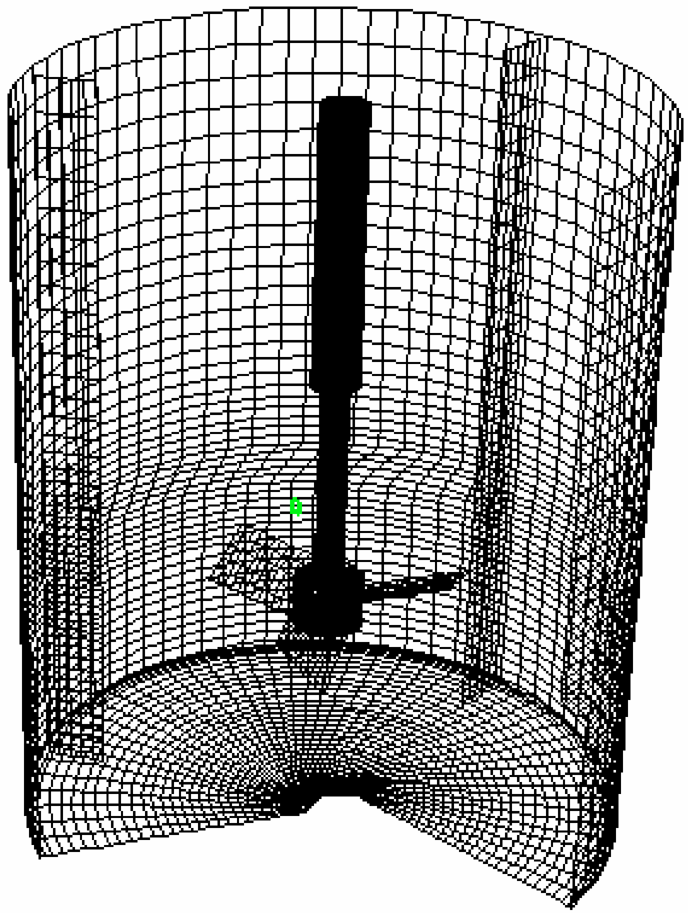


Fig. 1. Geometry and surface grid of the mixing tank. The rotor and two computational sectors of the tank are shown. The inlet in a one sector for the acid feed is shown as green.

CFD Results

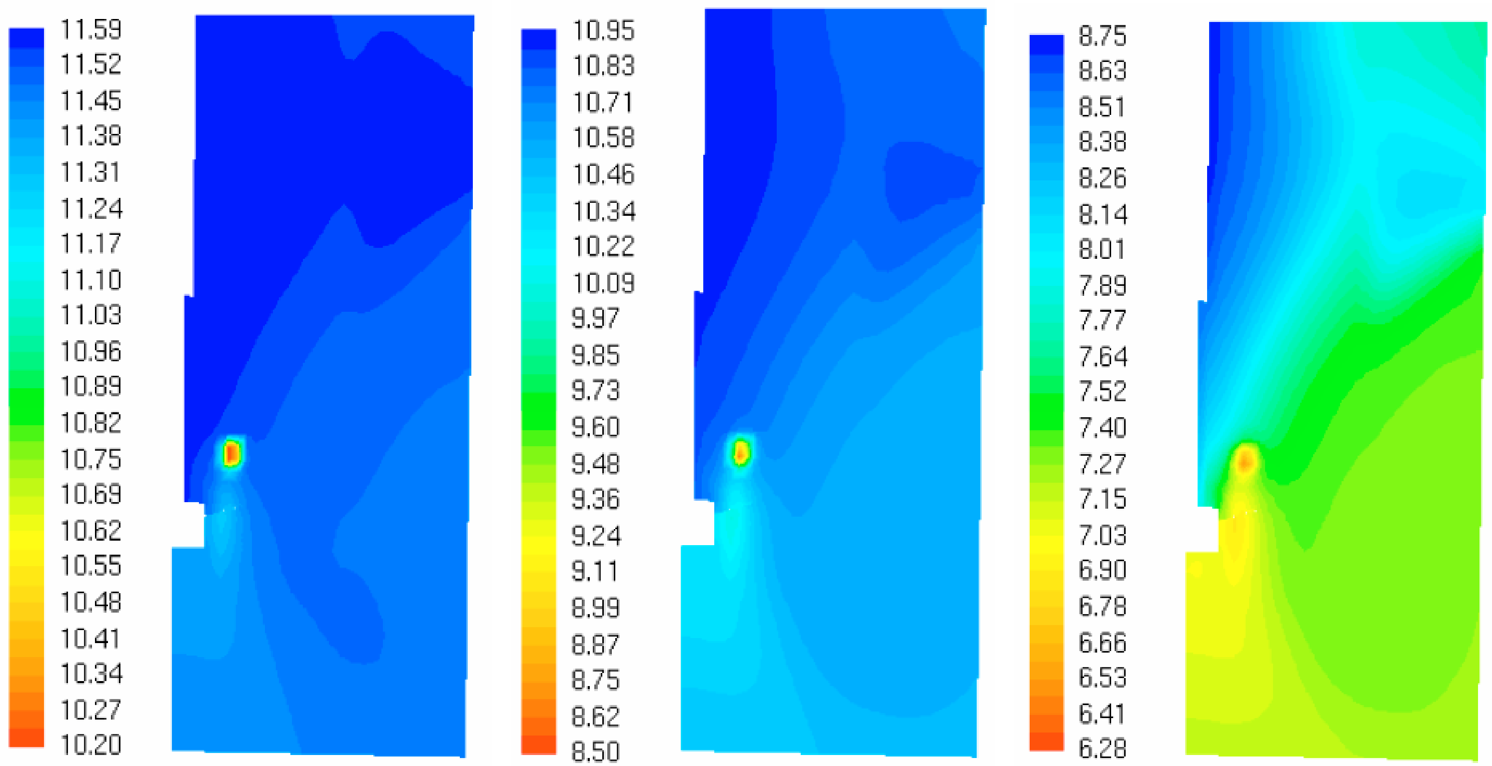


Fig. 2. Instant distribution of pH inside the mixing tank at the plane of acid feed inlet at the time 10 s, 50 s and 103 s. Note that for every figure the scale of the pH shown is different.