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In this project we will present the results of numerical simulations of chemical composition of flue gas produced by combustion of natural gas in an industrial heating device, i.e., a pusher furnace. In calculations of combustion chemistry, the CHEMKIN-PRO program was used. The gas-dynamic of flue gas was modeled with the use of the COMSOL Multiphysics program. In order to check the correctness of the plug flow reactor (PFR) model, as applied in calculations, a preliminary laboratory experiment was conducted. Based on measurement data that were obtained during the research on a laboratory stand, the boundary conditions were formulated and numerical simulations were carried out. The temperature and velocity profiles in the combustion chamber were determined with the use of the COMSOL program and were implemented in the CHEMKIN program. The obtained results of the numerical simulations performed in the experimental chamber showed high compliance with the results of measurements. This, in turn, led us to apply the analysis on a real object. The simulations of the chemical composition of flue gas in the

each zone of the furnace were carried out based on the measurements data collected from the real object, i.e., a pusher furnace that is currently working in one of the steel plants located in our country. CHEMKIN Pro (Chemical Kinetic Program) is an implicit, finite element (FE) non-equilibrium multiphase flow solver to obtain the concentration of species, vapor and liquid, for flow in any open geometry. It is used as a continuum solver for chemical kinetic modeling, for example, flame propagation, gas-phase chemistry, process kinetics, combustion, or underground gas migration, and as a discrete solver for chemical partitioning. The chemical kinetic equations are solved for each species in each zone of the flow geometry as a function of position, time, and species concentration.

During each time step, species mass fractions are calculated and species concentration gradients are determined. Pressure and velocity field are also updated on-the-fly if needed. CHEMKIN Pro can be used as a stand-alone program for single species problems or for multiphase flow problems that contain liquid or vapor components, or both liquid and vapor species. The boundary conditions are prescribed as prescribed flow or prescribed concentration profiles.

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we have included new tools in chemkin that can be used to validate the input parameters of reaction mechanisms. these tools are available in the examine tab of the workflow tab in chemkin. they can be used to check the mathematical correctness of the reaction mechanisms. chemkin-pro is a chemical kinetics simulator that models

idealized reacting flows and provides insight into results before production testing. relying on testing alone for verifying chemical processes is prohibitive, given today's shortened design cycles. effective simulation is critical for cost-effective designs and gets your product to market faster. i have updated iyers new janaf model to openfoam 1.7.x. in addition i have also updated the transport model. it now handles laminar viscosities of different species for temperatures up to 30000 k. the polynomials of the viscosities are still hard coded in the chemkin reader and contains only species which are interesting for arc welding applications. the polynomials are calculated with the transport model of our research group. today's energy standards call for high yields, efficiency and quality with minimal byproduct or waste. ansys chemkin-pro is a chemical kinetics simulator that models idealized reacting flows and provides insight into results before production testing. relying on testing alone for verifying chemical processes is prohibitive, given today's shortened design cycles. effective simulation is critical for cost-effective designs and gets your product to market faster. the last tab in chemkinlator is the time series tab. in this tab, one can create a time series using the reaction network previously defined and saved in chemkinlator. all the parameters (or the ranges of their values) that are defined in the reaction network are scanned in a user-defined interval of time. thus, chemkinlator creates a new simulation for each value of the parameter. the user can save the results of all the simulations in the form of an excel file that contains the time series of each reaction. once all the simulations are completed, the user can visually analyze the results to find which is the best performing reaction for a given experimental condition. 5ec8ef588b

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