% CSTR_ODE\CSTR_ODE_input1.m

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%
% This input file sets parameters for a steady state
% calculation of a single CSTR using the program CSTR_SS.m
%
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function [ProbDim,Reactor,Inlet,Physical,Rxn,StateInit,iflag] = ...
   CSTR_ODE_input1();

iflag = 0;


% Set reactor data
radius = 5;
height = 10;
Reactor.volume = height*pi*radius^2;
Reactor.F_vol = 20;

% Set the reactor temperature operation.
Reactor.nonisothermal = 1;
Reactor.T_cool = 1;
% The information below is only used in nonisothermal mode.
Reactor.F_cool = 1000;
Reactor.U_HT = 1000;
Reactor.A_HT = 2*pi*radius*height;
Reactor.Cp_cool = 1;

% Set number of species
ProbDim.num_species = 4;

% Set inlet concentrations and temperature
Inlet.conc = [1; 2; 0; 0];
Inlet.Temp = 1;

% Set the initial concentrations and temperature
StateInit.conc = [1; 2; 0; 0];
StateInit.Temp = 1;

% Set heat capacity data
Physical.Cp_data(1,:) = [1 0 0 0];
Physical.Cp_data(2,:) = [1 0 0 0];
Physical.Cp_data(3,:) = [1 0 0 0];
Physical.Cp_data(4,:) = [1 0 0 0];

% Set number of reactions
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ProbDim.num_rxn = 2;

% Allocate storage for reaction data
Rxn.stoich_coeff = zeros(ProbDim.num_rxn,ProbDim.num_species);
Rxn.ratelaw_exp = zeros(ProbDim.num_rxn,ProbDim.num_species);
Rxn.is_rxn_elementary = linspace(0,0,ProbDim.num_rxn)';
Rxn.k_ref = linspace(0,0,ProbDim.num_rxn)';
Rxn.T_ref = linspace(0,0,ProbDim.num_rxn)';
Rxn.E_activ = linspace(0,0,ProbDim.num_rxn)';
Rxn.delta_H = linspace(0,0,ProbDim.num_rxn)';

% Set reaction # 1 data
irxn = 1;
Rxn.stoich_coeff(irxn,:) = [-1 -2 1 0];
Rxn.is_rxn_elementary(irxn) = 0;
Rxn.ratelaw_exp(irxn,:) = [1 2 0 0];
Rxn.k_ref(irxn) = 1;
Rxn.T_ref(irxn) = 1;
Rxn.E_activ(irxn) = 1;
Rxn.delta_H(irxn) = -1;

% Set reaction # 2 data
irxn = 2;
Rxn.stoich_coeff(irxn,:) = [0 -1 -1 1];
Rxn.is_rxn_elementary(irxn) = 0;
Rxn.ratelaw_exp(irxn,:) = [0 1 1 0];
Rxn.k_ref(irxn) = 0.1;
Rxn.T_ref(irxn) = 1;
Rxn.E_activ(irxn) = 10;
Rxn.delta_H(irxn) = -1;


iflag = 1;

return;
```