Packbed program input data

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1 Input and output files

1. The Q2D model reads input data from the file 'input.dat'.
2. The solution is saved in output files 'molefractions_T_P_V.csv' and 'solution_T_P_V.csv'.
3. The file 'molefractions_T_P_V.csv' stores mole fractions of gas-phase species, density, pressure, temperature and surface coverages. T, P, and V corresponds to the inlet temperature, pressure and velocity (or flow rate).
4. The file 'solution_T_P_V.csv' stores the variables used in the solution vector (i.e. mass fractions of gas-phase species, density, pressure, temperature and surface coverages).
5. The CSV file starting with 'Err_' is saved in case of code failure. It saves the last successful steady-state solution.
6. The input file (input.dat) contains a parameter called 'RESTART' to specify if the user wants to use the previous solution as the initial guess.
7. If RESTART is set to 1, then the model reads the CSV file named 'savedSolution.csv' as the initial guess. The file 'savedSolution' gets saved every time the model is run.
8. To specify the initial guess from other file, specify 'INITGUESS_FROMFILE' to 1.

2 Input file keywords

The packed-bed reactor model reads the input data in a keyword format from the file named as 'input.dat'. Each keyword along with its corresponding values must appear on a separate line. There is no specific order for the keywords. The following tables provide a list of all keywords, their description and allowed values.

A list of all operating conditions required to run a simple reactor model is provided in Table 1. Table 2 tabulates filenames and phase-names of the chemistry mechanisms used for the lumen and the support catalysts. The advanced models such as energy, diffusion, and membrane related parameters are enlisted in Table 3. Finally, the BVP solver related parameters such as tolerances, grid refinement are described in Table 4.

Table 1: Operating conditions

INLETTEMP	Inlet Temperature [K]
OUTLETPRES	Outlet Pressure [Pa]
SCCM	Specify inlet flow rate in terms of [sccm]
VEL	Specify velocity in terms of [m/s]
SPECIESFRAC	Specify inlet composition in terms of MOLE/MASS-fractions [-]
SPECIESNAME	Value
SURF_SPECIESNAME	Value

Table 2: Input parameters for the reactor geometry

Parameters for the lumen	
POROSITY_LUMEN	Porosity of the bed [-]
TORTUOSITY_LUMEN	Tortuosity [-]
PARTICLEDIA_LUMEN	Particle Diameter [m]
PORERAD_LUMEN	Pore radius [m]
LENGTH_LUMEN	Length of the reactor [m]
CHANNELRAD_LUMEN	Radius of the reactor channel [m]
SPECIFICAREA_LUMEN	Catalyst specific area [1/m]
MICROPOROSITY_LUMEN	Porosity of micro-pores [-]
MICROPORERAD_LUMEN	Radius of micro-pores [m]
GASCTIFILE_LUMEN	Name of the YAML file containing gas phase
GASPHASE_LUMEN	Name of the gas phase in YAML file
SURFCTIFILE_LUMEN	Name of the YAML file containing surface phase
SURFPHASE_LUMEN	Name of the surface phase in YAML file
Parameters for the support	
POROSITY_SUPPORT	Porosity of the bed [-]
TORTUOSITY_SUPPORT	Tortuosity [-]
PARTICLEDIA_SUPPORT	Particle Diameter [m]
PORERAD_SUPPORT	Pore radius [m]
THICKNESS_SUPPORT	Thickness of the support [m]
CHANNELRAD_SUPPORT	Radius of the reactor channel [m]
SPECIFICAREA_SUPPORT	Catalyst specific area [1/m]
MICROPOROSITY_SUPPORT	Porosity of micro-pores [-]
MICROPORERAD_SUPPORT	Radius of micro-pores [m]
GASCTIFILE_SUPPORT	Name of the YAML file containing gas phase
GASPHASE_SUPPORT	Name of the gas phase in YAML file
SURFCTIFILE_SUPPORT	Name of the YAML file containing surface phase
SURFPHASE_SUPPORT	Name of the surface phase in YAML file
Parameters for the annular channel	
SOLVE_CHANNEL	Solve for annular channel [-]
CHANNELRAD_ANNULUS	Outer radius of the annular channel
CHANNEL_VEL	Inlet velocity inside the annular channel

Table 3: Advanced models in the packed-bed reactor code

	Energy equation
SOLVEENERGY	Solve Energy equation [1/0]
TWALL	Wall temperature
HCOEFF	Heat transfer coefficient
	Diffusion models
RAND_PORE_MODEL	Random pore model [0/1]
	Solid particle transport
COND_SOLID	Thermal conductivity of the solid Particle [W/m/K]
DENSITY_SOLID	Density of the solid Particle [kg/m^3]
CP_SOLID	Specific heat of the solid particle [J/kg/K]
EMISSIVITY	Emissivity
T_ENV	Environmental temperature [K]
A_ENV	Interface area of the porous media with surroundings
	Membrane parameters
MEMSOLVE	Include membrane flux [yes/no]
MEMSPNAME	Membrane-permeable species name
MEMTHICKNESS	Thickness of the membrane [m]
Ea_R	Ratio Ea/R for the membrane material [K]
k0	Permeability constant
SWEEPPRES	Sweep side pressure [Pa]

Table 4: Parameters for the boundary-value solver

	Solver controls
ATOL_SS	Absolute tolerance for steady solver
RTOL_SS	Relative tolerance for steady solver
ATOL_TS	Absolute tolerance for transient solver
RTOL_TS	Relative tolerance for transient solver
LOGLEVEL	Level of diagnostic output
MAXGRIDPOINTS	Maximum allowed grid points
MAXTIMESTEPS	Maximum number of time-steps allowed before successful steady-state solve
MINTIMESTEPS	Minimum number of time-steps allowed before successful steady-state solve
MAXTIMESTEPSIZE	Maximum time-step size
MINTIMESTEPSIZE	Minimum time-step size
	Mesh parameters
MESHPOINTS	Initial mesh points in axial direction
LUMEN_POINTS	Number of radial mesh points inside the lumen
SUPPORT_POINTS	Number of radial mesh points inside the support
REFINE	Refine the mesh [1/0]
MAX_GRID_RATIO	Value
MAX_DELTA	Value
MAX_DELTA_SLOPE	Value
PRUNE	Value