

*main.jl*

**Code generation**

Discretization  
Precomputing  
String parsing  
Symbolic computing  
Tracing jacobian

**Julia code**

*parm.jl*  
*cache.jl*  
*reactran.jl*  
*jactype.jl*

**&**

*ParsingDiagnostic.xlsx*

**Code execution**

**Initialization:**

ODE function  
Jacobian prototype  
Preconditioner  
Solver configuration  
Output configuration

**Code testing**

**Model run:**

Steady state simulation  
Transient simulation

**Model output**

*output.xlsx*  
*plots*

**Excel template**

*substances*  
*reactions*  
*parameters*  
*adsorption*  
*speciation*  
*options*  
*data*  
*output*