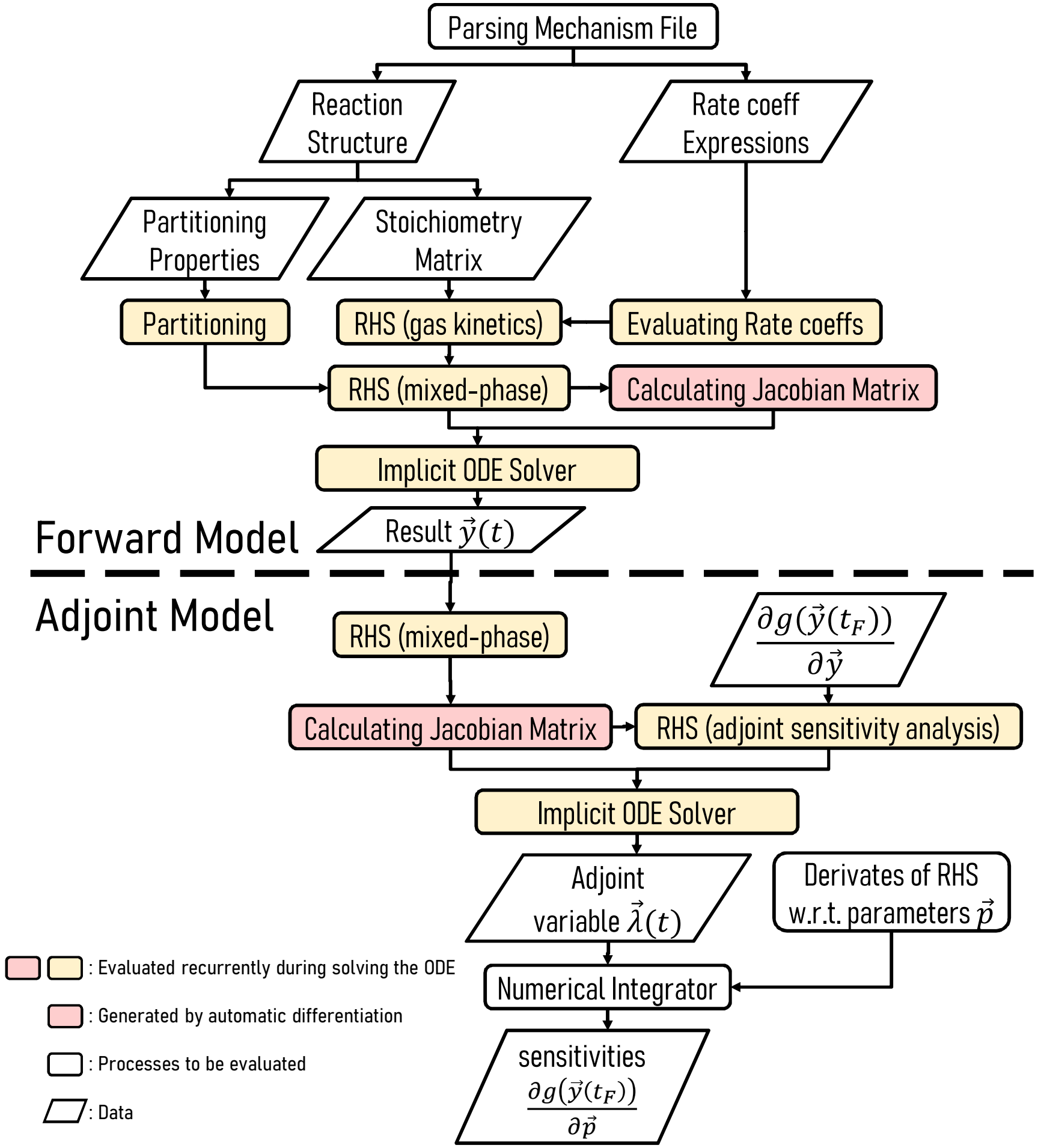
Parsing Mechanism File
Reaction Structure
Rate coeff Expressions
Partitioning Properties
Stoichiometry Matrix
Partitioning
RHS (gas kinetics)
Evaluating Rate coeffs
RHS (mixed-phase)
Calculating Jacobian Matrix
Implicit ODE Solver
Result $\vec{y}(t)$
Forward Model
Adjoint Model
RHS (mixed-phase)
$\frac{\partial g(\vec{y}(t_F))}{\partial \vec{y}}$
Calculating Jacobian Matrix
RHS (adjoint sensitivity analysis)
Implicit ODE Solver
Adjoint variable $\vec{\lambda}(t)$
Derivates of RHS w.r.t. parameters $\vec{p}$
Numerical Integrator
sensitivities $\frac{\partial g(\vec{y}(t_F))}{\partial \vec{p}}$
: Evaluated recurrently during solving the ODE
: Generated by automatic differentiation
: Processes to be evaluated
: Data