Mathematical modelling of processes in Chemical Engineering
MatLab quick-reference sheet

Algebraic equations (AE)	**Ordinary differential equations (ODE)**	**Differential-algebraic equations (DAE)**
	Mathematical formulation	
$\mathbf{f}(\mathbf{y}) = \mathbf{0}$	$\mathbf{y}' = \mathbf{f}(t, \mathbf{y})$ IC: $\mathbf{y}(0) = \mathbf{y}_0$	$\mathbf{F}(t, \mathbf{y}, \mathbf{y}') = \mathbf{0}$ IC: $\mathbf{y}(0) = \mathbf{y}_0$, $\mathbf{y}'(0) = \mathbf{y}'_0$
	Matlab model function header	
`function res=model(y,pars)`	`function yp=model(t,y,pars)`	`function res=model(t,y,yp,pars)`
	What to do before calling numerical algorithm function?	

`pars = [...];` set parameters
`yg = [...];` make guess
	`pars = [...];` set parameters
	`y0 = [...];` set IC
		`pars = [...];` set parameters
		`yg = [...]; ypg = [...]; fixed_y = [...];`
		`fixed_yp = [...]; [y0,yp0] = decic(@(t,y,yp)`
		`model(t,y,yp,pars), t0, yg, fixed_y, ypg, fixed_yp);`
		set IC and verify that IC are consistent

	Numerical algorithm function call	
`y = mmfsolve(@(y) model(y,pars), yg)`	`[tt,yy] = ode45(@(t,y) model(t,y,pars),` `[0,tend], y0)`	`[tt,yy] = ode15i(@(t,y,yp) model(t,y,yp,pars),` `[0,tend], y0, yp0)`
	What to do with results?	
`model(y,pars)`, verify that problem has converged to a solution	`plot(tt,yy(:,1),...)`, plot results	`plot(tt,yy(:,1),...)`, plot results
	Notes	
`mmfsolve` is not part of MatLab installation but must be downloaded from an open source. If MatLab installation contains optimization toolbox, it is recommended to use function `fsolve` instead.	An implicit solver, function `ode15s`, can be used for stiff systems.	

Partial differential equation (PDE) / Boundary value problem ODE
Finite volume method can be used to convert PDE to set of ODE (parabolic and hyperbolic PDE) or AE (elliptic PDE or boundary value problem ODE).