

button "Run Reaction" (id 35284)  
of stack "PFR With Heat Exchange"

```
on mouseEnter
  if the enabled of me is true then
    put "Click here to run an experiment." into temp
  else
    put "Not available now." into temp
  end if
  setInfo temp
end mouseEnter

# -----

on mouseUp

  global runCount
  global dataArray
  global runBeep
  global err

  setInfo empty

  put sciConv(line 1 of field "inputs") into k300
  put sciConv(line 2 of field "inputs") into Ea
  put sciConv(line 3 of field "inputs") into H
  put sciConv(line 4 of field "inputs") into dens
  put sciConv(line 5 of field "inputs") into capac
  put sciConv(line 6 of field "inputs") into Tin
  put sciConv(line 7 of field "inputs") into cin
  put sciConv(line 8 of field "inputs") into vol
  put sciConv(line 9 of field "inputs") into flow
  put sciConv(line 10 of field "inputs") into Tj
  put sciConv(line 11 of field "inputs") into U
  put sciConv(line 12 of field "inputs") into A

  put U*A into UA

  put vol/flow into tau
  put flow*cin into fa0 # inlet reactant molar flow rate

  # set initial conditions

  put cin into conc
  put zero into V
  put zero into conv
  put Tin into T

  # ... load input variables into line 1 of dataArray ...

  put empty into dataArray
  put format ("%10.3e", k300) into item 1 of line 1 of dataArray
  put format ("%10.3e", Ea) into item 2 of line 1 of dataArray
  put format ("%10.3e", H) into item 3 of line 1 of dataArray
  put format ("%10.3e", dens) into item 4 of line 1 of dataArray
  put format ("%10.3e", capac) into item 5 of line 1 of dataArray
  put format ("%10.3e", Tin) into item 6 of line 1 of dataArray
  put format ("%10.3e", cin) into item 7 of line 1 of dataArray
  put format ("%10.3e", vol) into item 8 of line 1 of dataArray
  put format ("%10.3e", flow) into item 9 of line 1 of dataArray
  put format ("%10.3e", Tj) into item 10 of line 1 of dataArray
  put format ("%10.3e", U) into item 11 of line 1 of dataArray
  put format ("%10.3e", A) into item 12 of line 1 of dataArray
  put format ("%10.3e", tau) into item 13 of line 1 of dataArray

  # ... also load output variables into line 1 ...

  put format ("%10.3e", V) into item 14 of line 1 of dataArray
```

button "Run Reaction" (id 35284)  
of stack "PFR With Heat Exchange"

```
put format ("%10.3e", conc) into item 15 of line 1 of dataArray
put format ("%10.3e", conv) into item 16 of line 1 of dataArray
put format ("%10.3e", T) into item 17 of line 1 of dataArray

# ... begin calculations specific to this lab ...

put dens*flow*capac into MC

# calc adiabatic delta T, positive for negative H (exothermic)
put -H*cin*flow/MC into deltaT

# calc max possible T
if H < 0 then # exothermic, deltaT is positive
  if Tj > Tin then
    put Tj + deltaT into maxT
  else
    put Tin + deltaT into maxT
  end if
else # endothermic
  if Tj > Tin then
    put Tj into maxT
  else
    put Tin into maxT
  end if
end if

# calc min possible T
if H > 0 then # endothermic, deltaT is negative
  if Tj < Tin then
    put Tj + deltaT into minT
  else
    put Tin + deltaT into minT
  end if
else # exothermic
  if Tj < Tin then
    put Tj into minT
  else
    put Tin into minT
  end if
end if
if minT < 0 then put 0 into minT

# integrate

put vol/100 into dv
put 0 into V
put 0 into i # step counter needed to initialize new line in dataArray
set cursor to watch

repeat while V <= vol

  add 1 to i
  if i > 1000 then exit repeat # don't want to compute too long

  put rk4(dv, k300, Ea, UA, Tj, vol, MC, H, cin, flow, conv, T) into temp # in stack script

  put item 1 of temp into dxdv
  put item 2 of temp into dTdv

  # make sure steps not too big
  repeat while abs(dv*dxdv) > 0.05 or abs(dv*dTdv) > 0.1
    put dv/2 into dv
    put rk4(dv, k300, Ea, UA, Tj, vol, MC, H, cin, flow, conv, T) into temp # in stack script
    put item 1 of temp into dxdv
    put item 2 of temp into dTdv
```

11:17 AM 5/8/18 2

button "Run Reaction" (id 35284)  
of stack "PFR With Heat Exchange"

**end repeat**

**# make sure steps not too small**

**repeat while**  $\text{abs}(\text{dv} \cdot \text{dxdv}) < 0.005$  **and**  $\text{abs}(\text{dv} \cdot \text{dTdv}) < 0.1$

**put**  $2 \cdot \text{dv}$  **into** dv

**if**  $2 \cdot \text{dv} > (\text{vol} - V)$  **then exit repeat**

**if**  $\text{conv} + \text{dv} \cdot \text{dxdv} > 0.9$  **then exit repeat**

**put** rk4(dv, k300, Ea, UA, Tj, vol, MC, H, cin, flow, conv, T) **into** temp **# in stack script**

**put item 1 of** temp **into** dxdv

**put item 2 of** temp **into** dTdv

**end repeat**

**put** conv + dv \* dxdv **into** conv

**if** conv > 0.99999 **then**

**put** 1 **into** conv

**else if** conv < 0 **then**

**put** 0 **into** conv

**end if**

**put** T + dv \* dTdv **into** T

**if** T > maxT **then**

**put** maxT **into** T

**else if** T < minT **then**

**put** minT **into** T

**end if**

**put** V + dv **into** V

**put** Cin \* (1 - conv) **into** conc

**# ... load next line of dataArray with results for this step ...**

**put empty into** line i+1 **of** dataArray **# need this to initialize the line!**

**put** format ("%10.3e", V) **into** item 14 **of** line i+1 **of** dataArray

**put** format ("%10.3e", conc) **into** item 15 **of** line i+1 **of** dataArray

**put** format ("%10.3e", conv) **into** item 16 **of** line i+1 **of** dataArray

**put** format ("%10.3e", T) **into** item 17 **of** line i+1 **of** dataArray

**end repeat**

**put the number of lines of** dataArray **into** runCount

**-- ... end of calculations specific to this lab ...**

**put** sciNote(conc) **into** line 1 **of** field "outputs"

**put** sciNote(conv) **into** line 2 **of** field "outputs"

**put** sciNote(T) **into** line 3 **of** field "outputs"

goodEnd

**end mouseUp**