# Application of Excel Macro Programming to Core Chemical Engineering Subjects

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# Motivation

- Our current chemical engineering curricula requires students to learn C++ in computer science.
- However, C++ will not be used further in their chemical engineering courses or their future working environment.
- Most chemical engineering graduates spend at least half of their workday at computer.
- Graduates work mostly involves the use of user-friendly commercial software (e.g. Excel).
- It is believed that it is more suitable to equip chemical engineering graduates with skills to use those commercial available software.

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# Project Aims

- This project aims to initiate the teaching of Excel VBA programming in chemical engineering.
- Teaching will be emphasized on the practical use of Excel VBA programming to solve chemical engineering problems.

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# Course Development (1)

- This course would initially be taught to first year students in the winter section.
- Teaching of Excel VBA programming will include self-learning, tutorial and practice.
- It is based on using practical examples in core courses, where students is required to write Excel VBA programs to solve practical chemical engineering problems.
- The use of Excel VBA was demonstrated to the students and compare with other methods of solution which could use (e.g. Excel spreadsheet or Polymath).

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# Course Development (2)

- Those examples and excises emphasis the power of using programming to replace time-consuming hand calculation, and the use of variable input / output as a generic solution to the problem.

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# Current Progress

- Course materials, examples are developed and test run at CENG 364 (Biomolecular Engineering) during the Spring semester 2007 and CENG 361 (Introduction to Biochemical Engineering) during the Fall semester 2007.
- The course is going to give to first year students in coming winter section / semester.

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# Example Program to Solve Chemical Engineering Problem

- This example is to demonstrate the advantage of writing own program as generic solution to chemical engineering problem.

- Fed-batch bioreactor is an example used in the Excel VBA programming course. It can demonstrate the benefit of using programming to replace inflexible solutions such as Polymath or spreadsheet.

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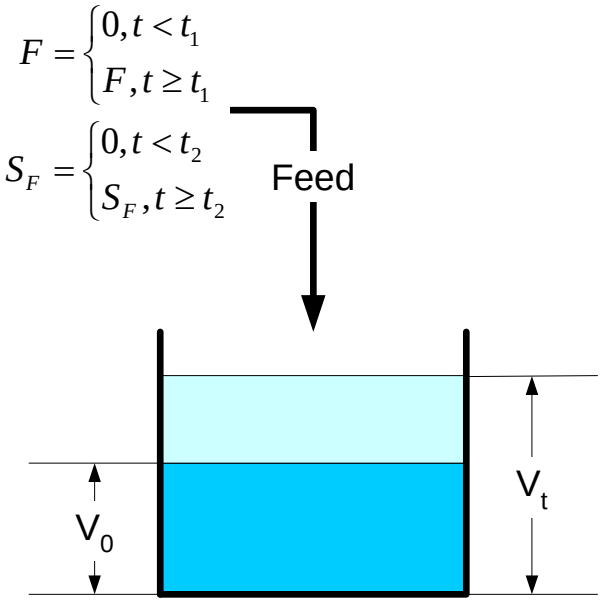
# Fed-Batch Bioreactor (1)

- A fed-batch bioreactor is a reactor that initially runs as a batch reactor, with volume $V_0$.
- After a certain period of time, a feed stream is introduced to input more substrate to maintain bacteria growth in the bioreactor.
- As the feed stream is introduced, the reactor volume changes from $V_0$ to $V_t$ with time.

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# Fed-Batch Reactor (2)

- Governing equations:

Specific growth rate: $$\mu_t = \mu_{\max} \frac{S_t}{K_S + S_t}$$

Reactor volume: $$\frac{dV_t}{dt} = F_t$$

Biomass: $$\frac{d(X_t \cdot V_t)}{dt} = X_t \cdot \frac{dV_t}{dt} + V_t \cdot \frac{dX_t}{dt} = X_t \cdot F_t + V_t \cdot (\mu \cdot X_t)$$

Substrate: $$\frac{d(S_t \cdot V_t)}{dt} = S_t \cdot \frac{dV_t}{dt} + V_t \cdot \frac{dS_t}{dt} = S_t \cdot F_t + V_t \cdot \left( F_t \cdot S_{F,t} - \frac{\mu \cdot X_t}{Y_{XS}} \right)$$

Product: $$\frac{d(P_t \cdot V_t)}{dt} = P_t \cdot \frac{dV_t}{dt} + V_t \cdot \frac{dP_t}{dt} = P_t \cdot F_t + V_t \cdot \left( \frac{\mu \cdot X_t \cdot Y_{PS}}{Y_{XS}} \right)$$

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# Fed-Batch Reactor (3)

- Governing equations (cont')

Feed rate: $$F = \begin{cases} 0, & 0 \le t < t_1 \\ F, & t \ge t_1 \end{cases}$$

Feed substrate conc.: $$S_F = \begin{cases} 0, & 0 \le t < t_1 \\ S_F, & t \ge t_1 \end{cases}$$

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# Fed-Batch Reactor (4)

- Initial condition:

Reactor volume: $V(t=0)=V_0$

Biomass level: $X(t=0)=X_0$

Substrate conc.: $S(t=0)=S_0$

Product conc.: $P(t=0)=P_0$

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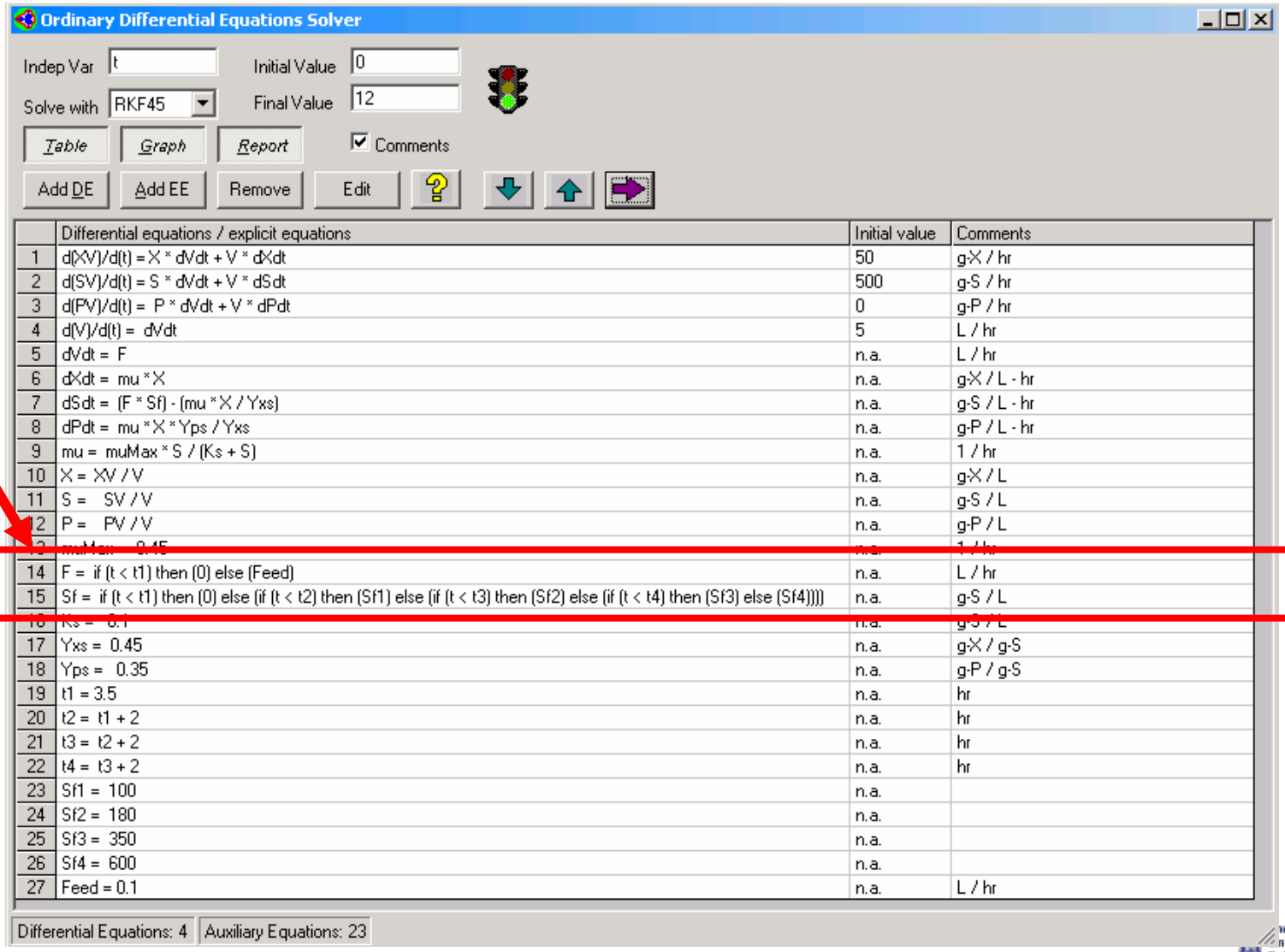
# Using Polymath (1)

Polymath file




| | Differential equations / explicit equations | Initial value | Comments |
|---|---|---|---|
| 1 | d(XV)/d(t) = X * dVdt + V * dXdt | 50 | g-X / hr |
| 2 | d(SV)/d(t) = S * dVdt + V * dSdt | 500 | g-S / hr |
| 3 | d(PV)/d(t) = P * dVdt + V * dPdt | 0 | g-P / hr |
| 4 | d(V)/d(t) = dVdt | 5 | L / hr |
| 5 | dVdt = F | n.a. | L / hr |
| 6 | dXdt = mu * X | n.a. | g-X / L - hr |
| 7 | dSdt = (F * Sf) - (mu * X / Yxs) | n.a. | g-S / L - hr |
| 8 | dPdt = mu * X * Yps / Yxs | n.a. | g-P / L - hr |
| 9 | mu = muMax * S / (Ks + S) | n.a. | 1 / hr |
| 10 | X = XV / V | n.a. | g-X / L |
| 11 | S = SV / V | n.a. | g-S / L |
| 12 | P = PV / V | n.a. | g-P / L |
| 13 | muMax = 0.45 | n.a. | 1 / hr |
| 14 | F = if (t < t1) then (0) else (Feed) | n.a. | L / hr |
| 15 | Sf = if (t < t1) then (0) else (if (t < t2) then (Sf1) else (if (t < t3) then (Sf2) else (if (t < t4) then (Sf3) else (Sf4)))) | n.a. | g-S / L |
| 16 | Ks = 0.1 | n.a. | g-S / L |
| 17 | Yxs = 0.45 | n.a. | g-X / g-S |
| 18 | Yps = 0.35 | n.a. | g-P / g-S |
| 19 | t1 = 3.5 | n.a. | hr |
| 20 | t2 = t1 + 2 | n.a. | hr |
| 21 | t3 = t2 + 2 | n.a. | hr |
| 22 | t4 = t3 + 2 | n.a. | hr |
| 23 | Sf1 = 100 | n.a. | |
| 24 | Sf2 = 180 | n.a. | |
| 25 | Sf3 = 350 | n.a. | |
| 26 | Sf4 = 600 | n.a. | |
| 27 | Feed = 0.1 | n.a. | L / hr |

Differential Equations: 4 | Auxiliary Equations: 23

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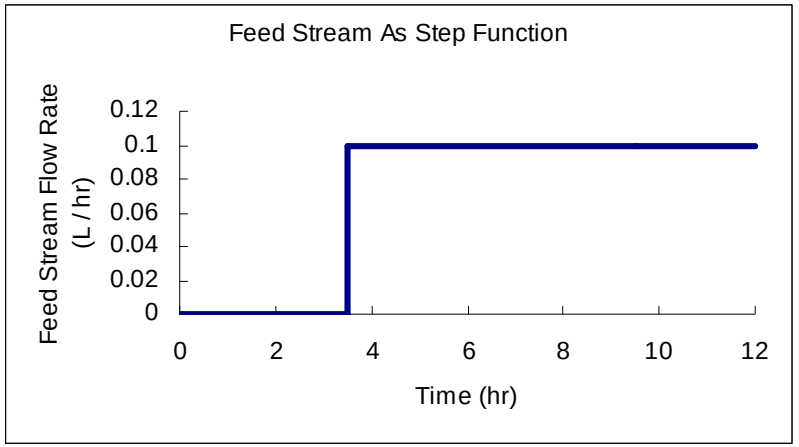
# Using Polymath (2)

- Step functions could be done by using the `IF-THEN-ELSE` statement to change value of constants according to simulation time:




```
F = IF ( time < 3.5 hr ) THEN (
            F = 0 L/hr
    ) ELSE (
            F = 0.1 L/hr
    )
```

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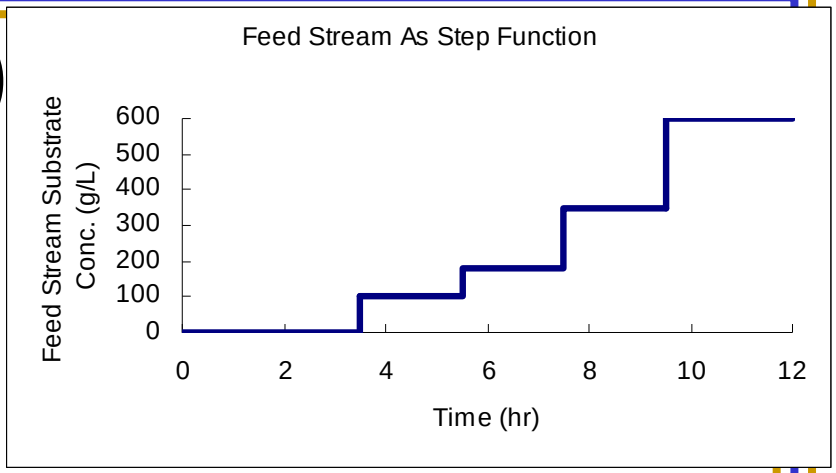
# Using Polymath (3)

- The multiple steps of feed substrate concentration could be done by using nested IF-THEN-ELSE statements:




- $S_{Feed}$ = IF ( time < 3.5 hr ) THEN (
  $S_{Feed}$ = 0 g/L
  ) ELSE ( IF ( time < 5.5 hr ) THEN (
  $S_{Feed}$ = 100 g/L
  ) ELSE ( IF ( time < 7.5 hr ) THEN (
  $S_{Feed}$ = 180 g/L
  ) ELSE ( IF ( time < 9.5 hr ) THEN
  $S_{Feed}$ = 350 g/L
  ) ELSE (
  $S_{Feed}$ = 600 g/L
  )
  )
  )
  )

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# Using Polymath (4)

- **Advantages:**
  - Polymath already built-in numerical integration methods;
  - Users only need to input differential equations, etc.
  - Step functions could be input by using the `IF ... THEN ... ELSE ...` statement provided by Polymath.

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# Using Polymath (5)

- **Disadvantages:**
  - Number of steps in step functions should be known before setting up the equations;
  - The numbers of nested `IF-THEN-ELSE` statements = number of steps - 1
  - If user wants to add more steps, he / she needs to modify the `IF-THEN-ELSE` statement, i.e. **no flexibility**;
  - Complicated `IF-THEN-ELSE` statements are not easy to read when there are many steps.
  - Polymath has limitation on the number of equations in a problem, for differential equation problems (Polymath version 6.10):

| Version | Educational | Professional |
|---|---|---|
| Max. # of simultaneous differential equations | 30 | 300 |
| Max. # of simultaneous explicit equations | 40 | 300 |
| Max. # of intermediate data points | 152 | 1200 |

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# Using Excel (1)

Spreadsheet file

- It is possible to set up an Excel spreadsheet with numerical integration methods.
- E.g. Reactor volume with feed stream:

| Step | Time | Vol | Feed |
|---|---|---|---|
| 0 | $t_0$ = 0 | $V_0$ | IF ( ( Time < 3.5 hr ), ( F = 0 ), ( F = 0.1 ) ) |
| 1 | $t_1$ = $t_0$ + h | $V_1$ = $V_0$ + F x h | IF ( ( Time < 3.5 hr ), ( F = 0 ), ( F = 0.1 ) ) |
| 2 | $t_2$ = $t_1$ + h | $V_2$ = $V_1$ + F x h | IF ( ( Time < 3.5 hr ), ( F = 0 ), ( F = 0.1 ) ) |
| 3 | $t_3$ = $t_2$ + h | $V_3$ = $V_2$ + F x h | IF ( ( Time < 3.5 hr ), ( F = 0 ), ( F = 0.1 ) ) |
| 4 | $t_4$ = $t_3$ + h | $V_4$ = $V_3$ + F x h | IF ( ( Time < 3.5 hr ), ( F = 0 ), ( F = 0.1 ) ) |

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# Using Excel (2)

- **Costs:**
  - Users need to set up their own numerical integration.
- **Advantages:**
  - Possible to perform numerical integration when no mathematical software package is available.
- **Disadvantages:**
  - The same style to input step functions as using Polymath, i.e. **no flexibility**.
  - Number of steps for numerical integration (i.e. number of rows in the spreadsheet) must be changed when the ending simulation time changes.

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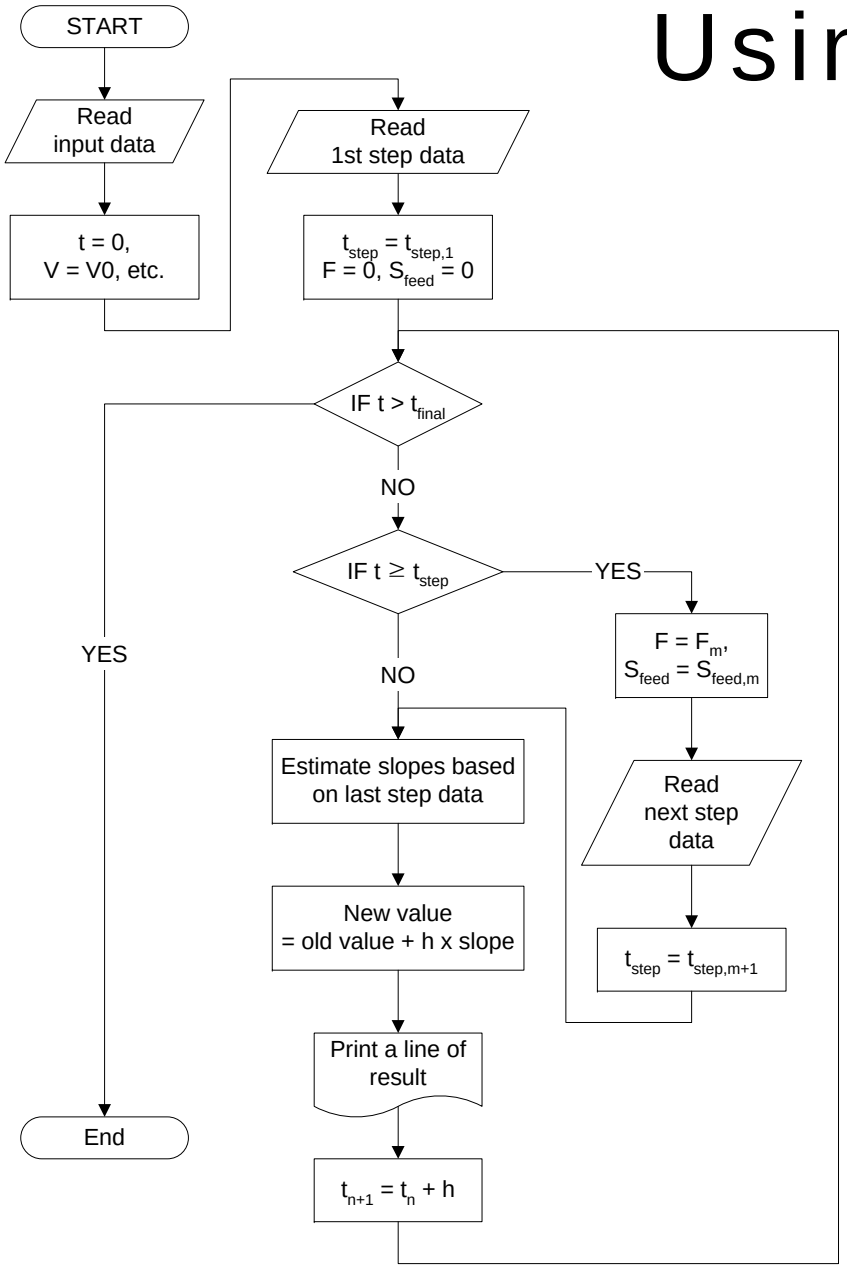
# Using Excel VBA (1)




- Numerical integration should be set up by user as VBA code.
- An automatic feed data reading code is introduced;
- It is possible to handle any number of steps.

Excel VBA file

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# Using Excel VBA (2)

- **Costs:**
  - Users need to write their own VBA program code.
- **Disadvantages:**
  - Need more time to set up the program;
  - Programming is not easy for novices.
- **Advantages:**
  - It is more flexible and can handle various kinds of decisions.
  - Although it requires time to set up the program, it is a one-off cost and this program can serve as generic solution towards this problem.

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# Excel VBA Project for Students

- In CENG 361 (Introduction to Biochemical Engineering), a project is given to student to let them to appreciate the benefit of the flexibility brought by write their own program.
- They are asked to write a program to solve sterilisation problem in the course.
- They are asked to develop an Excel spreadsheet solution and then write an Excel VBA program.  And to compare the benefit / advantages of either solution.

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