AUSTRALIAN JOURNAL OF BASIC AND APPLIED SCIENCES

ISSN:1991-8178 EISSN: 2309-8414
Journal home page: www.ajbasweb.com

Development of Equation Oriented Modelling of Advanced Distillation Process Using MOSAIC: Dividing Wall Column Case study

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ARTICLE INFO

Article history:
Received 18 September 2016
Accepted 21 January 2017
Available online 26 January 2017

Keywords:
Equation oriented modeling; dividing wall column; fatty acid separation; MOSAIC

ABSTRACT

This paper presents the development of an equation oriented models of chemical processes using MOSAIC. MOSAIC is a web-based modelling software developed by Dynamic and Operation of Technical Plants of TU Berlin. It provides a new platform which can be used as an alternative to the current approach of modeling using programing languages. MOSAIC is particularly useful in developing custom models of process unit operation that is not readily available in sequential modular based process simulators. MOSAIC allow users to develop models, generate the models' code and translate the model into different environments i.e. gPROMS, Aspen custom Modeler (ACM), Matlab etc. To shows its efficiency, a dividing wall column (DWC) for oleochemical fatty acid (FA) fractionation were modelled. A step by step approach to the modelling using MOSAIC is shown. The results are in agreement with data from steady state simulation in Aspen Plus and indicate that MOSAIC is a good modelling environment tool. Furthermore, the modelling effort is made possible even without the knowledge of programming languages. In addition, a comparison with another modelling environment (gProms, ACM, C++, Fortran) is highlighted which is useful in aiding researchers to choose MOSAIC for any modelling works.

INTRODUCTION

In process system engineering (PSE), the necessity to develop and to solve the customized models found an excellent response and there are numbers of mathematical software modelling tools that support the programming of equation-based models. Yet, the study of the workflow of models development and implementation shows massive obstacle like reduction of modelling errors and programming efforts, the avoidance of errors and effort in documentation (Kuntsche *et al.*, 2011). Modeling of chemical processes is usually done either using sequential modelling approach (SMA) or equation oriented (EO) programming. The former solves model block in the sequence given inlet streams. It is effective for large flow sheet, easy to use and user friendly. It is robust which ensure rigorous convergence and facilitate initialization step. Some examples are Aspen Plus, HYSYS, and Pro-II. Although the simulation can be done easily, it lacks in the transparency of equations systems involved and additional programming software such as Aspen Custom modeler (ACM) is needed to build customized equation oriented model (Stutzman *et al.*, 1982).

EO, on the other hand, solves a model of equations simultaneously. It is effective for solving heat-integrated or recycled processes, optimization and model tuning analysis. The equation oriented modelling of chemical processes has been done by using different modelling environments, these include gPROMS, ACM, GAMS, Matlab, C++, Fortran and so on. However, model formulation of custom models using such software is a time-consuming process since it takes a long time to write the programming language and debug the model. A limited of supported language makes the model is only applicable in an environment that comprehend the programming language of the model, for other environments, the model cannot be reusable and hence need to be re-programmed from scratch which requires a lot of programming effort. A further cause of error when programming the model associated with the visual distinction within mathematical expression in documentation and the calculation expression in the program code (Kuntsche, 2011). Hence, a new modelling environment called MOSAIC is applied in this study to develop customized model.

MOSAIC (www.mosaic-modelling.de) is a web-based equation oriented modelling environment for modelling of chemical processes. It is designed for minimization of modelling errors and programming effort, avoid programming errors, enhance file documentation and encouragement of cooperative data storage and sharing. As explained in Kuntsche *et al.* (2011), one of the important features of MOSAIC is modelling at the documentation level. The model equations in the documents i.e. books, journals etc. can be written easily in MOSAIC using TeX code. TeX is widely common and could be used by most of all researchers and generated a graphical good readable output of equations. Using TeX, the documented equations in MOSAIC have the same readability as the documentation itself. Therefore, modelling of equations can be done even without knowledge of any programming language.

As an example, we prefer to read a symbolic two-dimensional form,
$\alpha \cdot b = 3 \cdot (c + d)^{\beta}$
Rather than one dimensional form of a programming language,
Alpha*b = 3*pow (c + d, beta);

The uniqueness of MOSAIC compared with other software tools like Maple and MapleSim, which also allow collaborating with two-dimensional symbolic expression in this case is that, the variable names (refer figure 1) can contain a number of symbols that could be superscripted and subscripted (including several valued indices that may take a value or a range of value) (Kuntsche *et al*., 2011a).

In MOSAIC, modelling is done by creating objects separately. These objects include notation objects, equation objects, function objects, equation system objects, evaluation objects, and parameter objects. Notations are the fundamental modelling element in MOSAIC. Each variable contains in equations is provided with a notation that describes the meaning of the variable. Each object must be referring to a complete notation of all variables contained. Each object created in MOSAIC can be reused in another model since MOSAIC provide a good re-use facilities. This helps the user, for instance, to develop the notation suitable for the present project and apply it to all related models. Similarly with equations and equation systems. Thus, it will reduce the effort of modelling and allow reuse of model elements effectively. The other important feature of MOSAIC is code generation to other modelling environments i.e. Matlab, gPROMS, AMPL, ACM, GAMS, Modelica, etc. This is particularly useful especially for solving complex mathematical equations. MOSAIC itself can be a code generator and solver. In addition, MOSAIC also has the feature of centralized cooperation on the internet. It allows users to share their models easily in any computer and workstation. The shared model can be read or written on by another user on the internet.

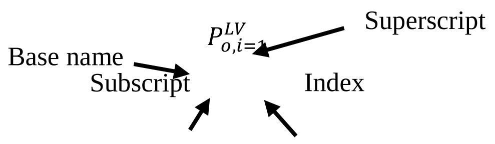


Fig. 1: Variable name in MOSAIC

The development and implementation of new models are hard and expensive task. This is because of the complexity and low reusability of process models (Mangold *et al*., 2002). Although with existence advanced modeling in the market, model formulation and configuration is still time consuming process in process modeling (Lam *et al*., 2007). To overcome some of the above mention EO modelling limitations, MOSAIC could provide a good alternative. Hence, the objective of this paper is twofold. First is to explore the modelling of DWC for fatty acid fractionation using MOSAIC. Second is to compare the features of MOSAIC with another modelling environment (gProms, ACM, GAMS, Matlab, C++, and Fortran). This could help in deciding to use MOSAIC for any modelling work.

Steady State Mathematical Modeling Of Dwc:

Previously, the modelling of DWC has been done by several researchers for dynamic and controllability purpose. However, all of them use a modelling environment tool based on the programming language such as Fortran (A. Woinaroschy, 2008), Matlab (Dohare *et al*., 2015), GAMS (Edna *et al*., 2016), and C++ (Kader, 2009). In this study, a new equation oriented approach (MOSAIC) is applied in modeling of DWC where the equations entered will be viewed in the form of symbolic mathematic expression.

Separation of the ternary and multicomponent system is applicable for dividing wall column (DWC). DWC is a single shell, fully thermal coupled distillation column which capable of separating mixtures of three and more components into high purity products. DWC has been known as an intensified alternative to conventional distillation separation of multicomponent mixtures, with reduced energy and capital cost. Basically, the column consists of four sections namely rectifying, pre-fractionator, middle, and stripping section as shown in Figure 2.

The first step of modeling begins by the formulation of equation models to describe the phenomenon occurring inside the distillation column. These formulated equations namely material balance equations, phase equilibrium equations, summation equations and heat balance equations or known as MESH equations will be required to formulate the model.

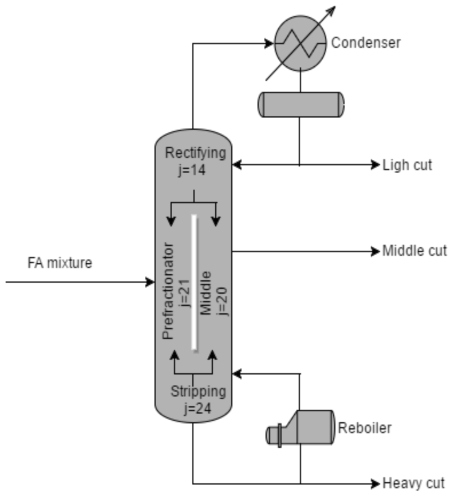


Fig. 2: DWC configuration for fatty acid fractionation (Illner and Othman, 2014)

MESH equations:

The principle of designing DWC models is based on a typical distillation column (DC). There are several models in modelling DC among others include steady-state equilibrium (EQ) stage model, dynamic EQ stage model, steady-state EQ stage model with stage efficiencies and dynamic EQ stage model with stage efficiencies (Baur, 2000). In this study, modelling of this model will be based on steady state EQ model. In EQ stage model, the vapor and liquid phases are assumed to be in thermodynamic equilibrium. The MESH equations used in this work are depicted from Dohare *et al*. (2015) and represented as below:-

Overall material balance (rectifying, pre-fractionation, middle and stripping section):

$$0 = V_{j+1}\, L_{j-1} - V_j - L_j + F_j - S_j \tag{1}$$

Component material balance for component *i* at stage *j* (refer figure 3):

$$0 = V_{j+1,} y_{j+1,} L_{j-1} x_{j-1,i} - V_j y_{j,i} - L_j x_{j,i} + F_j z_{j,i} - S_j x_{j,i} \tag{2}$$

Since the model is assumed as steady state, and thus the derivative of material balance will be equal zero. Both *j* and *i* are subscripts to represent the stages numbers and components respectively. *F* represents feed flow rate, *S* represent side stream flow rate, *L* represents liquid flow rate, and *V* will represent vapor flow rate. *x* and *y* are the mole fraction of liquid and vapor respectively. While *z* represent the feed composition. The total liquid holdup on each stage is assumed unity (neglect flow dynamics).

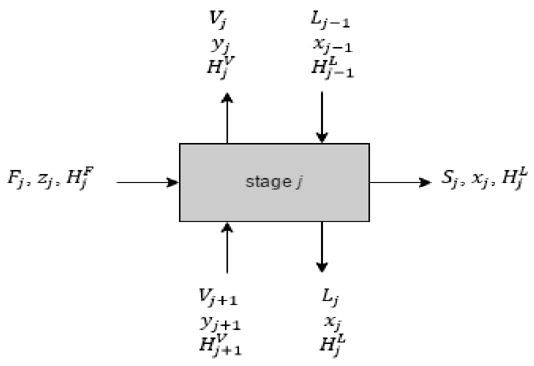


Fig. 3: Material balance diagram for stage *j*

Phase equilibrium equations:

Phase equilibrium relation equation describes the relationship between liquid mole fraction and vapor mole fraction of chemical components when vapor and liquid at equilibrium state. For the ideal condition, the value of activity coefficient, γ will be equal to 1. Saturated vapor pressure, P^o can be calculated using Antoine equation and P is the pressure of the column.

$$y_{j,i} = K_{j,i}x_{j,i} \qquad \text{where } K_{j,i} = \frac{\gamma_{j,i} P^o_{j,i}}{P_j} \tag{3}$$

Summation equations:

The summation equation states that sum of mole fraction of each component in the liquid phase and vapor phase of each stage which is equal to 1.

$$\sum_{i=1}^{N} x_{j,i} = 1 \qquad \sum_{i=1}^{N} y_{j,i} = 1 \tag{4}$$

Energy balance equations:

The energy balance of each stage of DWC can be described by the following equation:

$$0 = V_{j+1}H^V_{j+1} + L_{j-1}H^L_{j-1} - V_jH^V_j - L_jH^L_j + F_jH^F_j - S_jH^L_j \tag{5}$$

In energy balance, H^L_j and H^V_j represent the liquid and vapor enthalpy on the j th stage, respectively. Again, for the steady state, the derivative of energy balance will be equal to zero.

Internal flow in DWC:

The challenge in DWC modelling is to accommodate the internal flow between the partition walls. Based on figure 1, the partition wall in the middle of the column (section 3) separates the pre-fractionator (section 2) and the middle section. A feed stream is introduced into the pre-fractionator section while the side stream removes the intermediate component from the middle section. Liquid from rectifying section (section 1) will be split into two parts, some portion enters the pre-fractionator section and the rest, to the middle section. The liquid splitting can be described by an equation as follow:

$$r^{(2)} = \alpha L^{(1)}_{n1} \qquad \text{where } \alpha \text{ is liquid split factor} \tag{6}$$

$$r^{(3)} = (1-\alpha)L^{(1)}_{n1} \tag{7}$$

On the other hand, vapor from stripping column (section 4) is also split into both pre-fractionator and middle section according to the following equations:

$$V^{(2)}_{n2} = \beta V^{(4)}_{1} \qquad \text{where } \beta \text{ is vapour split factor} \tag{8}$$

$$V^{(3)}_{n3} = (1-\beta)V^{(4)}_{1} \tag{9}$$

At the intersection of rectifying section with pre-fractionator section and middle section, the vapor is mixed according to the following equations:

$$V^{(1)}_{n1} = V^{(2)}_{1} + V^{(3)}_{1} \tag{10}$$

$$V^{(1)}_{n1} y^{(1)}_{n1,i} = V^{(2)}_{1} y^{(2)}_{1,i} + V^{(3)}_{1} y^{(3)}_{1,i} \tag{11}$$

Whereas, at the intersection of the pre-fractionator section and a middle section with stripping section 4, the liquid mixing can be described as follows:

$$r^{(4)} = r^{(2)}_{n2} + r^{(3)}_{n3} \tag{12}$$

$$r^{(4)}x^{(4)}_{r} = r^{(2)}_{n2}x^{(2)}_{n2} + r^{(3)}_{n3}x^{(3)}_{n3} \tag{13}$$

DWC process description:

The DWC in this work is used to separate fatty acid cuts into three products namely light cut (LC), middle cut (MC), and heavy cut (HC). The design parameters for the DWC is based on the work by Illner and Othman (2014) in which the rectifying section consists of 14 stages, while pre-fractionator section have 21 stages, middle section and stripping section have 20 and 24 stages respectively. The condenser is at stage 0 and reboiler at the last/bottom stage of the column. The operating pressure is 0.03 bar. Feed stream enters at stage 10 from the top in the pre-fractionator section and the side product is withdrawn at stage 3 in middle section. Details of the DWC design and feed specifications are shown in Table 1. Illner and Othman (2014) have simulated the process in Aspen Plus using the equivalent model of DWC with four rigorous RADFRAC model, two unit of mixers and splitters for the liquid and vapour internal mixing and splitting purpose. The Aspen results will be utilized for initialization value in MOSAIC and comparison purposes.

Table 1: Summary of the DWC design specifications

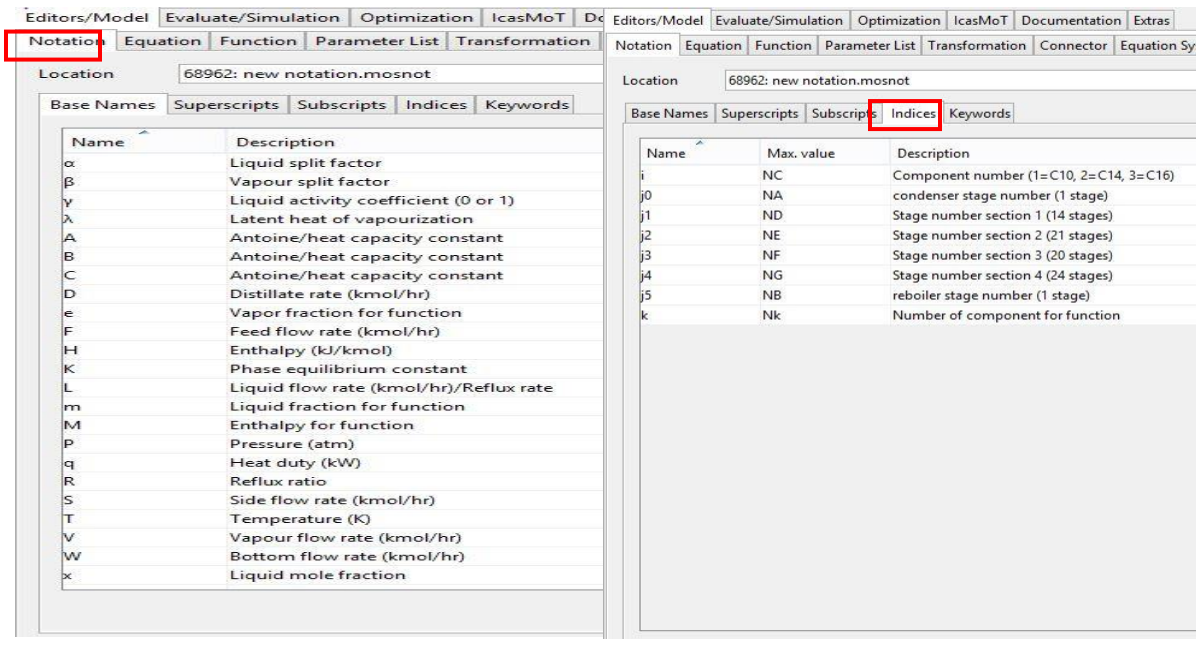
Parameter	Specification
Feed stream	FA mixture
Feed flow rate (kmol/hr)	0.02187
Temperature (K)	448.15
Column pressure (bar)	0.03
Feed composition (mass fraction)	
• C10 (LC)	0.085
• C14 (MC)	0.65
• C16 (HC)	0.265
Liquid split factor	0.84
Vapour split factor	0.5
No of stages (Rectifying/Pre-frac/Middle/Stripping)	14/21/20/24

Steps For Modeling In Mosaic:

The steps of modelling using MOSAIC is summarized in Figure 7. Overall there are seven steps.

Step 1: Creation of a notation:

In this first step, symbols with descriptions are created in the Notation page to represent all variables involve in the equations as shown in Figure 4. Each variable is represented by a unique base name or can be attached together with subscripts and/or superscripts. By introducing subscripts/superscripts, two or more variables are allowed to have a similar base name. Additionally, indices involved in the equations can also be added. Note that, all notations should have a unique description such as its full abbreviation or engineering units.



Location 68962: new notation.mosnot

Name	Description
α	Liquid split factor
β	Vapour split factor
γ	Liquid activity coefficient (0 or 1)
λ	Latent heat of vapourization
A	Antoine/heat capacity constant
B	Antoine/heat capacity constant
C	Antoine/heat capacity constant
D	Distillate rate (kmol/hr)
e	Vapor fraction for function
F	Feed flow rate (kmol/hr)
H	Enthalpy (kJ/kmol)
K	Phase equilibrium constant
L	Liquid flow rate (kmol/hr)/Reflux rate
m	Liquid fraction for function
M	Enthalpy for function
P	Pressure (atm)
q	Heat duty (kW)
R	Reflux ratio
S	Side flow rate (kmol/hr)
T	Temperature (K)
V	Vapour flow rate (kmol/hr)
W	Bottom flow rate (kmol/hr)
x	Liquid mole fraction

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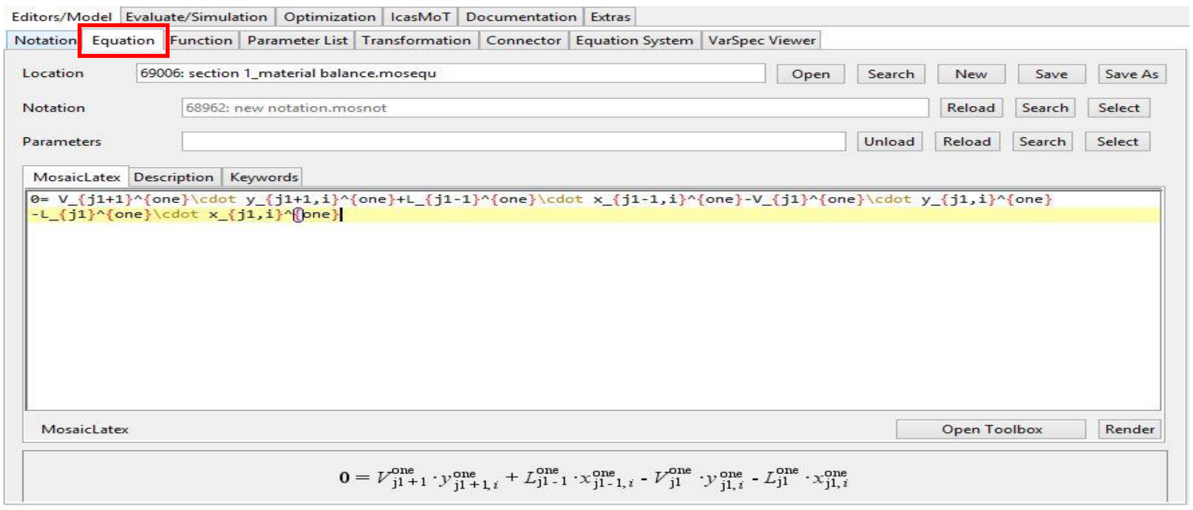
Name	Max. value	Description
i	NC	Component number (1=C10, 2=C14, 3=C16)
j0	NA	condenser stage number (1 stage)
j1	ND	Stage number section 1 (14 stages)
j2	NE	Stage number section 2 (21 stages)
j3	NF	Stage number section 3 (20 stages)
j4	NG	Stage number section 4 (24 stages)
j5	NB	reboiler stage number (1 stage)
k	Nk	Number of component for function

Fig. 4: Notation declaration screenshot from the MOSAIC GUI

Step 2: Creation of equation objects:

The next step is to create the equations. The equations formulation can be written using a TeX-style mathematical language as shown in Figure 5. TeX is a documentary language which allows equations to be expressed in mathematical terms. When creating the equation, it might also have a parameter list to emphasize variables that should be treated as global parameters. However, for this case, all equations does not involve a parameter (refer step 3 for creating parameter list). Note that when using subscripts or superscripts, curly brackets are compulsory. All operators, have to be expressed clearly and any missing operators could cause an error. For instance, to express '*V times y is equal to 0*', the expression is supposed to be *V* . y=0, not *Vy=0* as the second expression could be easily be misunderstood as *'variable Vy is equal to 0*'.



Location: 69006: section 1_material balance.mosequ

Notation: 68962: new notation.mosnot

Parameters:

```
0= V_{j1+1}^{one}\cdot y_{j1+1,i}^{one}+L_{j1-1}^{one}\cdot x_{j1-1,i}^{one}-V_{j1}^{one}\cdot y_{j1,i}^{one}
-L_{j1}^{one}\cdot x_{j1,i}^{one}
```

$$0 = V_{j1+1}^{one} \cdot y_{j1+1,i}^{one} + L_{j1-1}^{one} \cdot x_{j1-1,i}^{one} - V_{j1}^{one} \cdot y_{j1,i}^{one} - L_{j1}^{one} \cdot x_{j1,i}^{one}$$

Fig. 5: Mathematical equations creation

Step 3: Creation of function objects:

Step 3 is almost the same as the creation of equation objects. However, the method of creating functions is not as straightforward as creating equations which may require the creation of parameter list objects. Functions usually consist of one output value and several input values. A function is required whenever it is possible to compute the value of an output variable that is dependent on a finite number of input variables in the equation system. Besides, the notation of a function is independent and unrelated from the notation used in the equation system. An example in this case study to create saturated pressure function using Antoine equation is as follows (please refer Figure 6):-

i) The parameter for Antoine equation is first created by loading the 'notation of parameter.mosnot' in notation file.

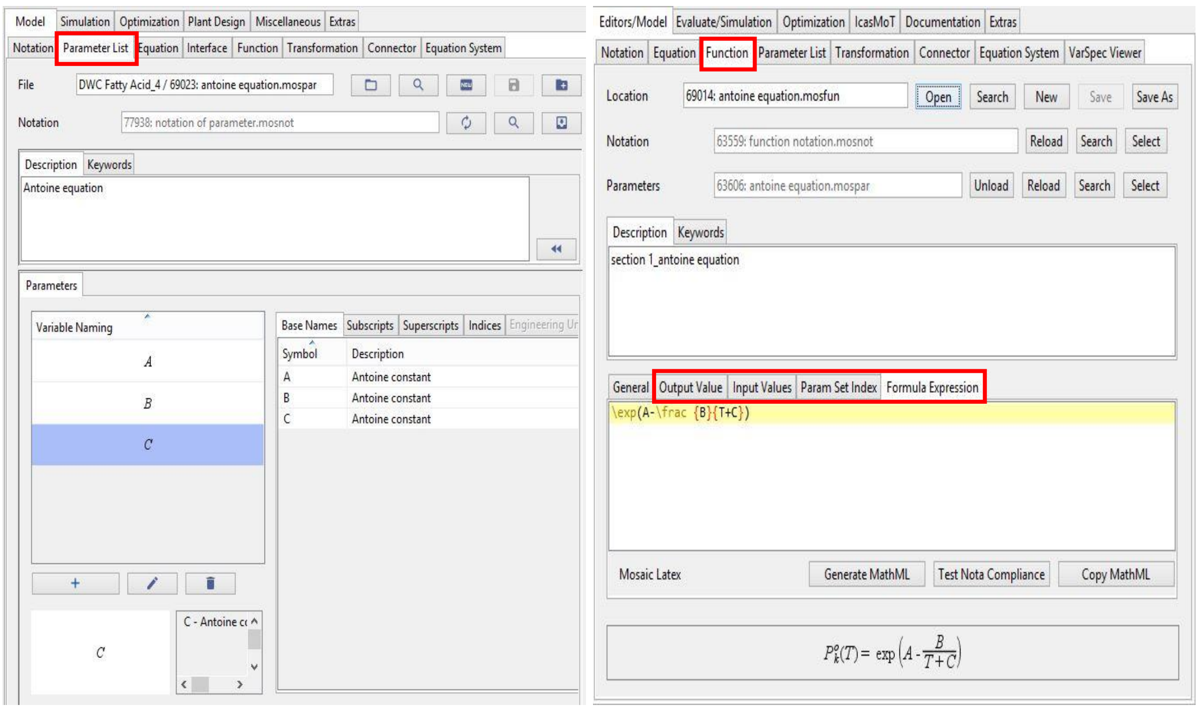
ii) Next, create and save the parameter list (A, B, and C) as 'antoine equation'. Note that, the list of parameters does not have any index. They are considered as a special form of design variable and are kept in a separate list in the degree of freedom calculation.

iii) Then, create the function by loading the 'antoine equation.mospar' in the parameters file, and 'function notation.mosnot' in the notation file as well.

iv) Click and insert the output variable (P^o) and input variable (T) in output/input tab.

v) After that, activate the 'param set index' tab to specify which index of the parameter list's notation is used if the function is applied with an index. In this case, "k" is used which indicate the component index ($k = 3$).

vi) Finally, express the right-hand side of the equation in the formula expression tab and save the function.



File: DWC Fatty Acid_4 / 69023: antoine equation.mospar

Notation: 77938: notation of parameter.mosnot

Antoine equation

Variable Naming
A
B
C

Symbol	Description
A	Antoine constant
B	Antoine constant
C	Antoine constant

C C - Antoine co

Location: 69014: antoine equation.mosfun

Notation: 63559: function notation.mosnot

Parameters: 63606: antoine equation.mospar

section 1_antoine equation

```
\exp(A-\frac {B}{T+C})
```

$$P_k^o(T) = \exp\left(A - \frac{B}{T+C}\right)$$

Fig. 6: Parameter list and function creation.

Step 4: Creation of equation systems:

After all equations and functions have been defined, it needs to be connected by equation systems. Adding equations and functions to equation systems can be done easily. First of all, the notation must be loaded before creating the equation system. Then, in the connected elements tab, all equations and equation systems that have created will be added by clicking 'add' button as shown in Figure 8(a). Next is to add the function. It is required to set the input variables and its corresponding output variable. Noted that in Figure 8(b) the 'Input Naming' and 'Output Naming' in the function itself are called 'Generic Naming', while the corresponding variables in the equation system are termed 'Applied Naming'. For this case, P^o and T will be applied as $P_{j1,i}^{o,one}$ (saturated pressure of the i th component at the j th stage in section 1) of DWC and T_{j1}^{one} (temperature at the j th stage in section 1) respectively. A preview of all equations and functions in an equation system can be generated as shown in Figure 8(a).

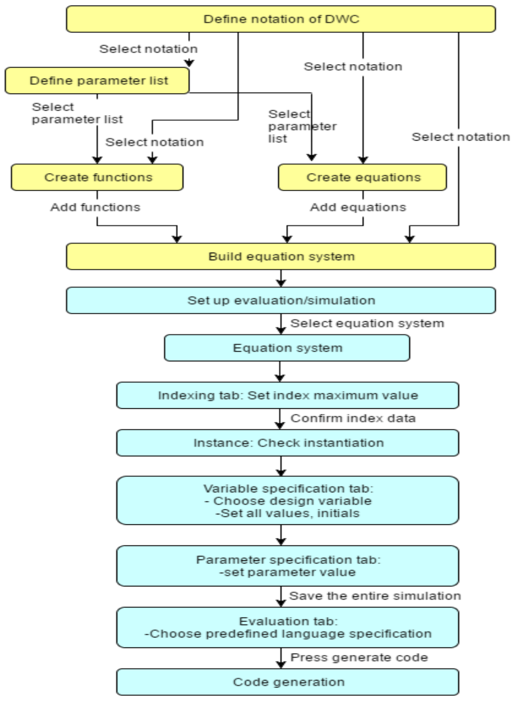
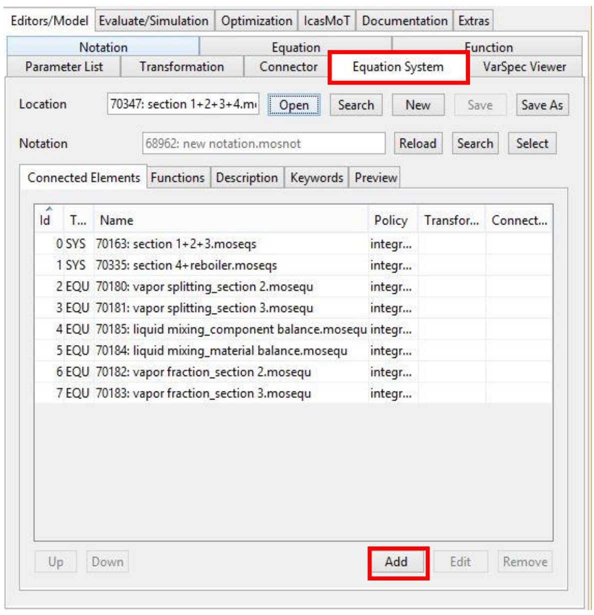


Fig. 7: Procedure of modelling using MOSAIC

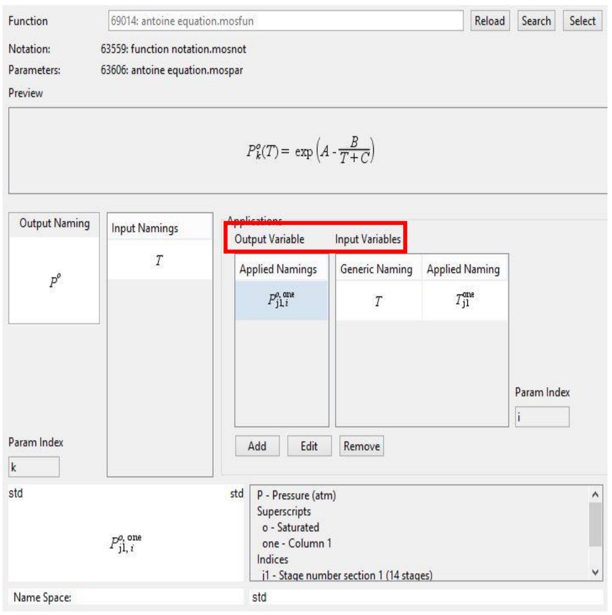


Location: 70347: section 1+2+3+4.m

Notation: 68962: new notation.mosnot

Id	T...	Name	Policy	Transfor...	Connect...
0	SYS	70163: section 1+2+3.moseqs	integr...		
1	SYS	70335: section 4+reboiler.moseqs	integr...		
2	EQU	70180: vapor splitting_section 2.mosequ	integr...		
3	EQU	70181: vapor splitting_section 3.mosequ	integr...		
4	EQU	70185: liquid mixing_component balance.mosequ	integr...		
5	EQU	70184: liquid mixing_material balance.mosequ	integr...		
6	EQU	70182: vapor fraction_section 2.mosequ	integr...		
7	EQU	70183: vapor fraction_section 3.mosequ	integr...		

(a)



Function: 69014: antoine equation.mosfun

Notation: 63559: function notation.mosnot

Parameters: 63606: antoine equation.mospar

$$P^o_k(T) = \exp\left(A - \frac{B}{T+C}\right)$$

Output Naming: P^o

Input Namings: T

Applied Namings: $P^{o,\,one}_{j1,i}$

Generic Naming	Applied Naming
T	T^{one}_{j1}

Param Index: k

Param Index: i

std $P^{o,\,one}_{j1,\,i}$

std
P - Pressure (atm)
Superscripts
o - Saturated
one - Column 1
Indices
j1 - Stage number section 1 (14 stages)

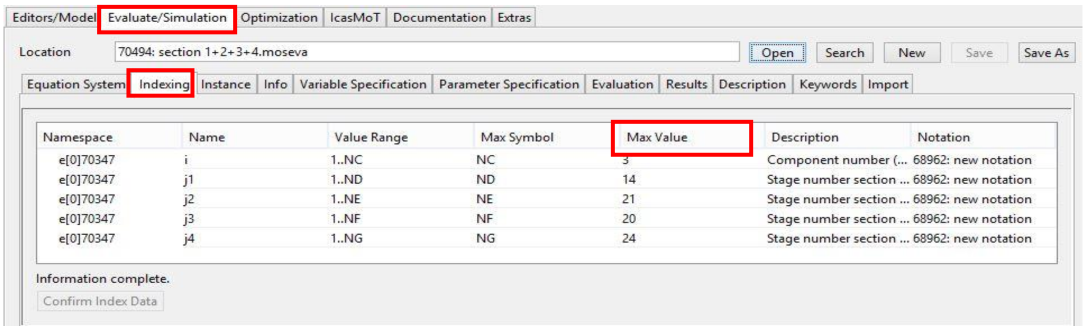
Name Space: std

(b)

Fig. 8: Equation system editor of (a) connected elements/equations and (b) functions

Step 5: Creation of evaluation objects:

Once equation systems have been created, an evaluation object is then created. The purpose of evaluation object is to provide all necessary information to specify a problem to be solved based on the equation system. This includes specification of the maximum index value, classification of design and iteration variables, and giving values to the design and parameter variables as well as providing initial values for the iteration variables. In order to create the evaluation objects, the equation system first has to be loaded. Once it is loaded, indexing can be made by specifying the max value of each index shown in figure 9(a). Once specified, all equations and functions involved in the model are generated and shown in the 'Instance' as in Figure 9(b).

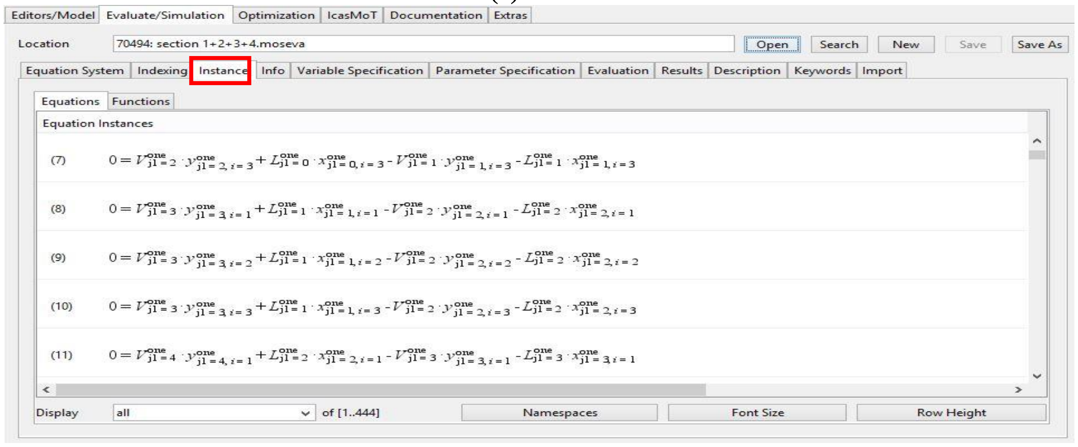


Location: 70494: section 1+2+3+4.moseva

Namespace	Name	Value Range	Max Symbol	Max Value	Description	Notation
e[0]70347	i	1..NC	NC	3	Component number (...	68962: new notation
e[0]70347	j1	1..ND	ND	14	Stage number section ...	68962: new notation
e[0]70347	j2	1..NE	NE	21	Stage number section ...	68962: new notation
e[0]70347	j3	1..NF	NF	20	Stage number section ...	68962: new notation
e[0]70347	j4	1..NG	NG	24	Stage number section ...	68962: new notation

Information complete.

(a)



Location: 70494: section 1+2+3+4.moseva

Equation Instances

(7) $0 = V^{one}_{j1=2} \cdot y^{one}_{j1=2,\,i=3} + L^{one}_{j1=0} \cdot x^{one}_{j1=0,\,i=3} - V^{one}_{j1=1} \cdot y^{one}_{j1=1,\,i=3} - L^{one}_{j1=1} \cdot x^{one}_{j1=1,\,i=3}$

(8) $0 = V^{one}_{j1=3} \cdot y^{one}_{j1=3,\,i=1} + L^{one}_{j1=1} \cdot x^{one}_{j1=1,\,i=1} - V^{one}_{j1=2} \cdot y^{one}_{j1=2,\,i=1} - L^{one}_{j1=2} \cdot x^{one}_{j1=2,\,i=1}$

(9) $0 = V^{one}_{j1=3} \cdot y^{one}_{j1=3,\,i=2} + L^{one}_{j1=1} \cdot x^{one}_{j1=1,\,i=2} - V^{one}_{j1=2} \cdot y^{one}_{j1=2,\,i=2} - L^{one}_{j1=2} \cdot x^{one}_{j1=2,\,i=2}$

(10) $0 = V^{one}_{j1=3} \cdot y^{one}_{j1=3,\,i=3} + L^{one}_{j1=1} \cdot x^{one}_{j1=1,\,i=3} - V^{one}_{j1=2} \cdot y^{one}_{j1=2,\,i=3} - L^{one}_{j1=2} \cdot x^{one}_{j1=2,\,i=3}$

(11) $0 = V^{one}_{j1=4} \cdot y^{one}_{j1=4,\,i=1} + L^{one}_{j1=2} \cdot x^{one}_{j1=2,\,i=1} - V^{one}_{j1=3} \cdot y^{one}_{j1=3,\,i=1} - L^{one}_{j1=3} \cdot x^{one}_{j1=3,\,i=1}$

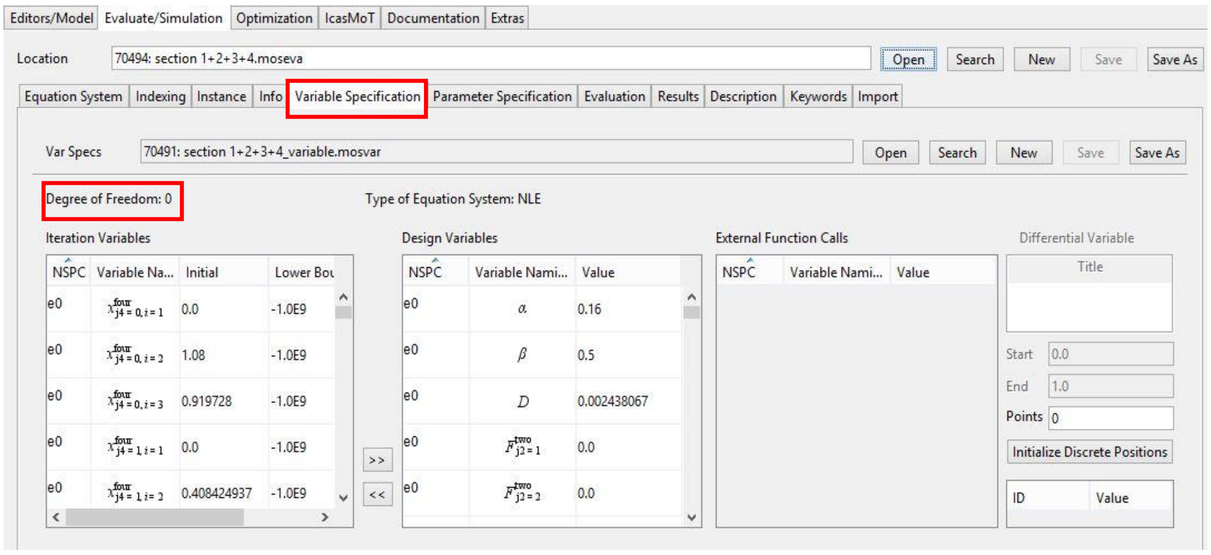
Display: all of [1..444]

(b)

Fig. 9: (a) Index specification and (b) list of equations in the system

Step 6: Specification of initial values and design values:

The next step is to define iteration variables and design variables. Generally, fixed value variables are design variables whereas calculated variables are iteration variables. The degree of freedom (DOF) will be automatically calculated until it becomes zero which giving the DOF for the actual selection of design variables and does consider linear independency (refer figure 10). The value of each design variable must be specified. For the iteration variables, good initial values are important in solving the models since the modelling would work well when all variables are near the solution(Pantelides *et al*., 2015; Aspen Technology, 2009). Thus, in this case study, all initialization values were based on the results of Aspen Plus steady state simulation data for good convergence. In this case study, the temperature and liquid composition of eah stage in every section ($T_{j1}^{one}, T_{j2}^{two}, T_{j3}^{three}, T_{j4}^{four}, x_{j1}^{one}, x_{j2}^{two}, x_{j3}^{three}, x_{j4}^{four}$) will be assigned as an iteration variables. In addition, the parameters specification values that contain in the equation system need to be specified as well. The entire simulation (equation system, indexing, variable and parameter speification) need to be save prior to evaluation.



Location 70494: section 1+2+3+4.moseva

Var Specs 70491: section 1+2+3+4_variable.mosvar

Degree of Freedom: 0

Type of Equation System: NLE

Iteration Variables

NSPC	Variable Na...	Initial	Lower Bou
e0	$x_{j4=0,i=1}^{four}$	0.0	-1.0E9
e0	$x_{j4=0,i=2}^{four}$	1.08	-1.0E9
e0	$x_{j4=0,i=3}^{four}$	0.919728	-1.0E9
e0	$x_{j4=1,i=1}^{four}$	0.0	-1.0E9
e0	$x_{j4=1,i=2}^{four}$	0.408424937	-1.0E9

Design Variables

NSPC	Variable Nami...	Value
e0	α	0.16
e0	β	0.5
e0	D	0.002438067
e0	$F_{j2=1}^{two}$	0.0
e0	$F_{j2=2}^{two}$	0.0

External Function Calls

NSPC	Variable Nami...	Value

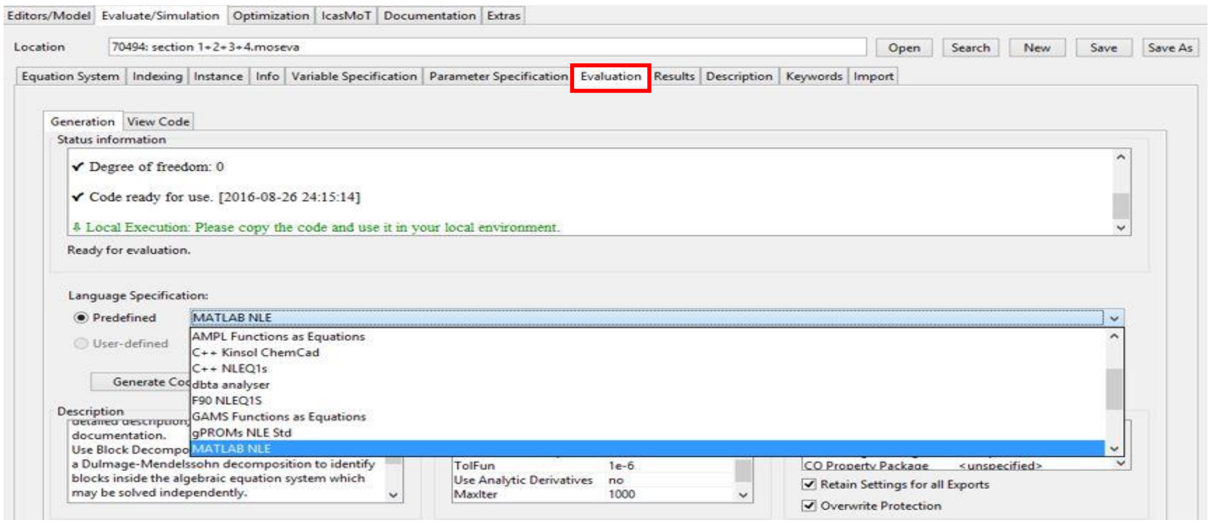
Start 0.0
End 1.0
Points 0

ID	Value

Fig. 10: Variable specifications of equation system

Step 7: Code generation and evaluation:

The concept of MOSAIC is to provide code generation for many languages. In this work, the selection for code generation is MATLAB NLE (Nonlinear Equation System) (refer figure 11). On the tab generation, status information which contains a checklist of the steps to be accomplished right before code generation. In case the information is not complete, hints (text saying either information missing or ready for evaluation) are shown. The generated codes can be run at their own corresponding environment for the solving of the model. Figure 12 shows a portion of the whole codes. The code is then compiled in Matlab.



Location 70494: section 1+2+3+4.moseva

Status information

✓ Degree of freedom: 0

✓ Code ready for use. [2016-08-26 24:15:14]

⇓ Local Execution: Please copy the code and use it in your local environment.

Ready for evaluation.

Language Specification:

[✓ Predefined] MATLAB NLE

User-defined

AMPL Functions as Equations
C++ Kinsol ChemCad
C++ NLEQ1s
dbta analyser
F90 NLEQ1S
GAMS Functions as Equations
gPROMs NLE Std
MATLAB NLE

Description

detailed description, documentation.
Use Block Decompo
a Dulmage-Mendelssohn decomposition to identify blocks inside the algebraic equation system which may be solved independently.

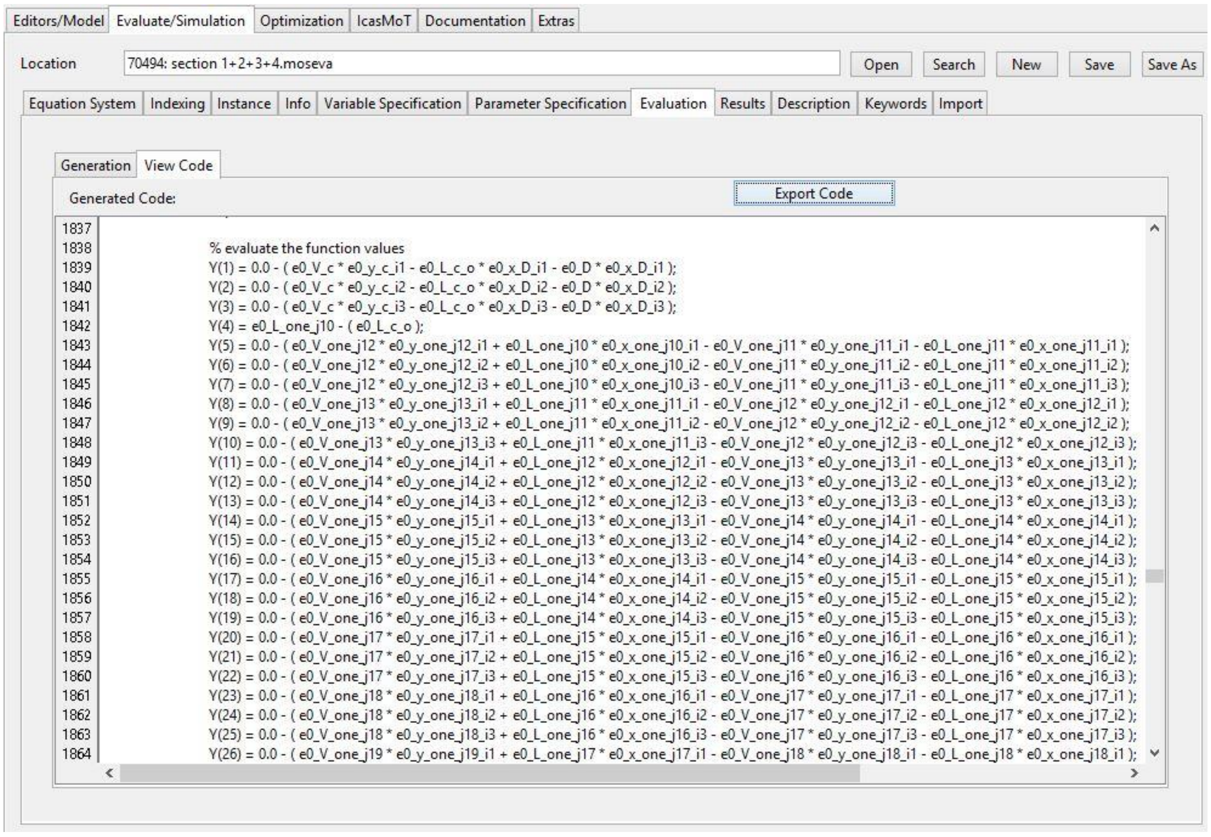
TolFun	1e-6
Use Analytic Derivatives	no
MaxIter	1000

CO Property Package <unspecified>

✓ Retain Settings for all Exports

✓ Overwrite Protection

Fig. 11: Code generation and evaluation



```
% evaluate the function values
Y(1) = 0.0 - ( e0_V_c * e0_y_c_i1 - e0_L_c_o * e0_x_D_i1 - e0_D * e0_x_D_i1 );
Y(2) = 0.0 - ( e0_V_c * e0_y_c_i2 - e0_L_c_o * e0_x_D_i2 - e0_D * e0_x_D_i2 );
Y(3) = 0.0 - ( e0_V_c * e0_y_c_i3 - e0_L_c_o * e0_x_D_i3 - e0_D * e0_x_D_i3 );
Y(4) = e0_L_one_j10 - ( e0_L_c_o );
Y(5) = 0.0 - ( e0_V_one_j12 * e0_y_one_j12_i1 + e0_L_one_j10 * e0_x_one_j10_i1 - e0_V_one_j11 * e0_y_one_j11_i1 - e0_L_one_j11 * e0_x_one_j11_i1 );
Y(6) = 0.0 - ( e0_V_one_j12 * e0_y_one_j12_i2 + e0_L_one_j10 * e0_x_one_j10_i2 - e0_V_one_j11 * e0_y_one_j11_i2 - e0_L_one_j11 * e0_x_one_j11_i2 );
Y(7) = 0.0 - ( e0_V_one_j12 * e0_y_one_j12_i3 + e0_L_one_j10 * e0_x_one_j10_i3 - e0_V_one_j11 * e0_y_one_j11_i3 - e0_L_one_j11 * e0_x_one_j11_i3 );
Y(8) = 0.0 - ( e0_V_one_j13 * e0_y_one_j13_i1 + e0_L_one_j11 * e0_x_one_j11_i1 - e0_V_one_j12 * e0_y_one_j12_i1 - e0_L_one_j12 * e0_x_one_j12_i1 );
Y(9) = 0.0 - ( e0_V_one_j13 * e0_y_one_j13_i2 + e0_L_one_j11 * e0_x_one_j11_i2 - e0_V_one_j12 * e0_y_one_j12_i2 - e0_L_one_j12 * e0_x_one_j12_i2 );
Y(10) = 0.0 - ( e0_V_one_j13 * e0_y_one_j13_i3 + e0_L_one_j11 * e0_x_one_j11_i3 - e0_V_one_j12 * e0_y_one_j12_i3 - e0_L_one_j12 * e0_x_one_j12_i3 );
Y(11) = 0.0 - ( e0_V_one_j14 * e0_y_one_j14_i1 + e0_L_one_j12 * e0_x_one_j12_i1 - e0_V_one_j13 * e0_y_one_j13_i1 - e0_L_one_j13 * e0_x_one_j13_i1 );
Y(12) = 0.0 - ( e0_V_one_j14 * e0_y_one_j14_i2 + e0_L_one_j12 * e0_x_one_j12_i2 - e0_V_one_j13 * e0_y_one_j13_i2 - e0_L_one_j13 * e0_x_one_j13_i2 );
Y(13) = 0.0 - ( e0_V_one_j14 * e0_y_one_j14_i3 + e0_L_one_j12 * e0_x_one_j12_i3 - e0_V_one_j13 * e0_y_one_j13_i3 - e0_L_one_j13 * e0_x_one_j13_i3 );
Y(14) = 0.0 - ( e0_V_one_j15 * e0_y_one_j15_i1 + e0_L_one_j13 * e0_x_one_j13_i1 - e0_V_one_j14 * e0_y_one_j14_i1 - e0_L_one_j14 * e0_x_one_j14_i1 );
Y(15) = 0.0 - ( e0_V_one_j15 * e0_y_one_j15_i2 + e0_L_one_j13 * e0_x_one_j13_i2 - e0_V_one_j14 * e0_y_one_j14_i2 - e0_L_one_j14 * e0_x_one_j14_i2 );
Y(16) = 0.0 - ( e0_V_one_j15 * e0_y_one_j15_i3 + e0_L_one_j13 * e0_x_one_j13_i3 - e0_V_one_j14 * e0_y_one_j14_i3 - e0_L_one_j14 * e0_x_one_j14_i3 );
Y(17) = 0.0 - ( e0_V_one_j16 * e0_y_one_j16_i1 + e0_L_one_j14 * e0_x_one_j14_i1 - e0_V_one_j15 * e0_y_one_j15_i1 - e0_L_one_j15 * e0_x_one_j15_i1 );
Y(18) = 0.0 - ( e0_V_one_j16 * e0_y_one_j16_i2 + e0_L_one_j14 * e0_x_one_j14_i2 - e0_V_one_j15 * e0_y_one_j15_i2 - e0_L_one_j15 * e0_x_one_j15_i2 );
Y(19) = 0.0 - ( e0_V_one_j16 * e0_y_one_j16_i3 + e0_L_one_j14 * e0_x_one_j14_i3 - e0_V_one_j15 * e0_y_one_j15_i3 - e0_L_one_j15 * e0_x_one_j15_i3 );
Y(20) = 0.0 - ( e0_V_one_j17 * e0_y_one_j17_i1 + e0_L_one_j15 * e0_x_one_j15_i1 - e0_V_one_j16 * e0_y_one_j16_i1 - e0_L_one_j16 * e0_x_one_j16_i1 );
Y(21) = 0.0 - ( e0_V_one_j17 * e0_y_one_j17_i2 + e0_L_one_j15 * e0_x_one_j15_i2 - e0_V_one_j16 * e0_y_one_j16_i2 - e0_L_one_j16 * e0_x_one_j16_i2 );
Y(22) = 0.0 - ( e0_V_one_j17 * e0_y_one_j17_i3 + e0_L_one_j15 * e0_x_one_j15_i3 - e0_V_one_j16 * e0_y_one_j16_i3 - e0_L_one_j16 * e0_x_one_j16_i3 );
Y(23) = 0.0 - ( e0_V_one_j18 * e0_y_one_j18_i1 + e0_L_one_j16 * e0_x_one_j16_i1 - e0_V_one_j17 * e0_y_one_j17_i1 - e0_L_one_j17 * e0_x_one_j17_i1 );
Y(24) = 0.0 - ( e0_V_one_j18 * e0_y_one_j18_i2 + e0_L_one_j16 * e0_x_one_j16_i2 - e0_V_one_j17 * e0_y_one_j17_i2 - e0_L_one_j17 * e0_x_one_j17_i2 );
Y(25) = 0.0 - ( e0_V_one_j18 * e0_y_one_j18_i3 + e0_L_one_j16 * e0_x_one_j16_i3 - e0_V_one_j17 * e0_y_one_j17_i3 - e0_L_one_j17 * e0_x_one_j17_i3 );
Y(26) = 0.0 - ( e0_V_one_j19 * e0_y_one_j19_i1 + e0_L_one_j17 * e0_x_one_j17_i1 - e0_V_one_j18 * e0_y_one_j18_i1 - e0_L_one_j18 * e0_x_one_j18_i1 );
```

Fig. 12: Generated code in MOSAIC

Model Comparison With Aspen Plus:

Upon running in MATLAB and converged, the temperature profile of the DWC model is shown in Figure 13. In the rectifying section, it can be seen that temperature is maintained at 440 K and starts to increase slowly to 494 K and 484 K in the pre-fractionation and middle section respectively. The temperature difference between these two sections is 10 K. Column temperature continues to increase until it achieves the temperature of 503 K at the stripping section. For composition profile, the results are shown in Figure 14. The system reached nearly 99% purity of C10 (LC) on distillate product, 94% of C14 (MC) on side product, and 99% of C16 (HC) on the bottom product. Upon comparing with results of Aspen Plus, as in Table 2, it can be seen that the expected results of code generated (temperature and product composition) by MOSAIC are in agreement with the data taken from simulation results. This proves that MOSAIC is indeed a great modelling environment tool due to good functionality in code generator to another different language. Besides, this indicates that the equations of the DWC model formulated in MOSAIC are precise and reliable. In addition, the extended work in dynamic behavior and control structure of DWC can be develop using the steady-state results of MOSAIC.

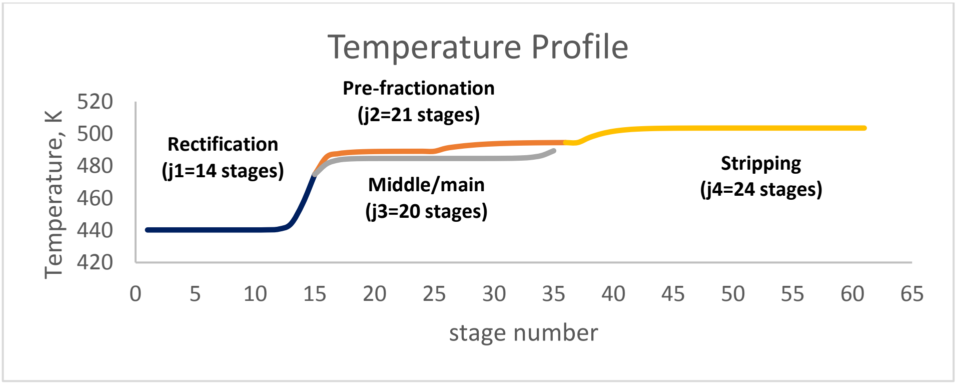
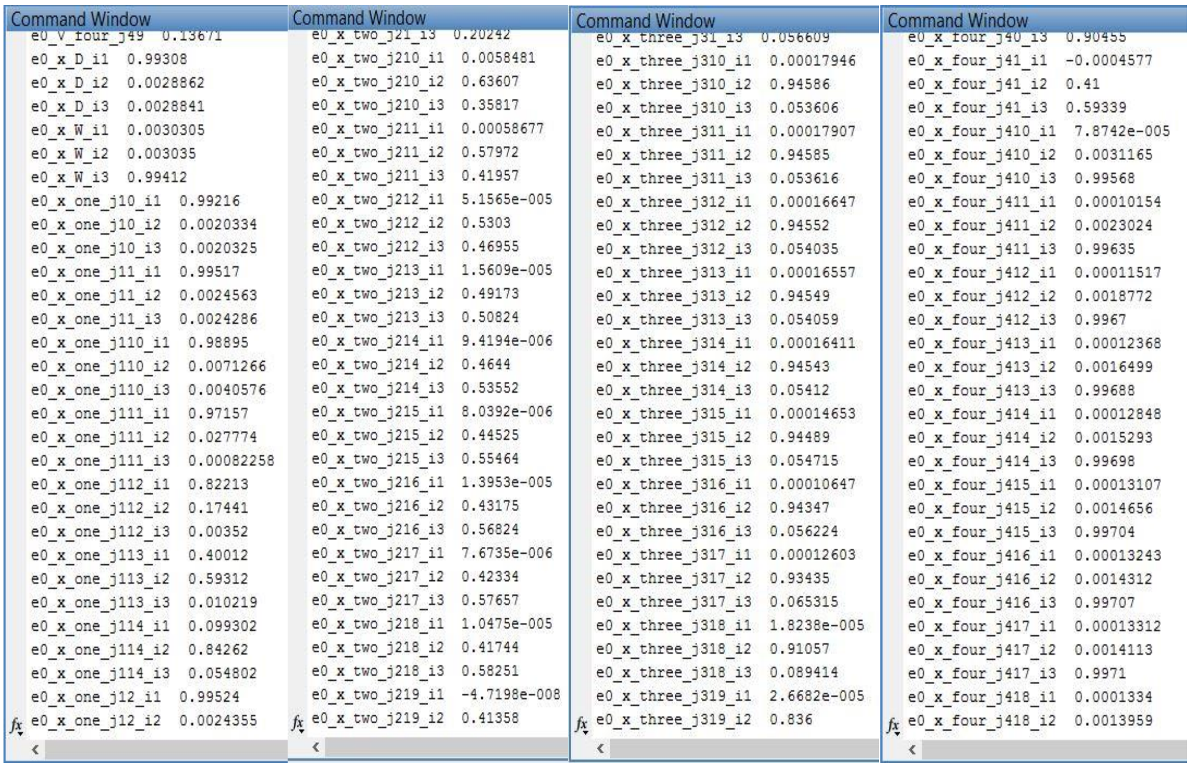


Fig. 13: Temperature versus stage number in each section



```
e0_V_four_j49   0.13671
e0_x_D_i1  0.99308
e0_x_D_i2  0.0028862
e0_x_D_i3  0.0028841
e0_x_W_i1  0.0030305
e0_x_W_i2  0.003035
e0_x_W_i3  0.99412
e0_x_one_j10_i1  0.99216
e0_x_one_j10_i2  0.0020334
e0_x_one_j10_i3  0.0020325
e0_x_one_j11_i1  0.99517
e0_x_one_j11_i2  0.0024563
e0_x_one_j11_i3  0.0024286
e0_x_one_j110_i1  0.98895
e0_x_one_j110_i2  0.0071266
e0_x_one_j110_i3  0.0040576
e0_x_one_j111_i1  0.97157
e0_x_one_j111_i2  0.027774
e0_x_one_j111_i3  0.00082258
e0_x_one_j112_i1  0.82213
e0_x_one_j112_i2  0.17441
e0_x_one_j112_i3  0.00352
e0_x_one_j113_i1  0.40012
e0_x_one_j113_i2  0.59312
e0_x_one_j113_i3  0.010219
e0_x_one_j114_i1  0.099302
e0_x_one_j114_i2  0.84262
e0_x_one_j114_i3  0.054802
e0_x_one_j12_i1  0.99524
e0_x_one_j12_i2  0.0024355
```

```
e0_x_two_j21_i3   0.20242
e0_x_two_j210_i1  0.0058481
e0_x_two_j210_i2  0.63607
e0_x_two_j210_i3  0.35817
e0_x_two_j211_i1  0.00058677
e0_x_two_j211_i2  0.57972
e0_x_two_j211_i3  0.41957
e0_x_two_j212_i1  5.1565e-005
e0_x_two_j212_i2  0.5303
e0_x_two_j212_i3  0.46955
e0_x_two_j213_i1  1.5609e-005
e0_x_two_j213_i2  0.49173
e0_x_two_j213_i3  0.50824
e0_x_two_j214_i1  9.4194e-006
e0_x_two_j214_i2  0.4644
e0_x_two_j214_i3  0.53552
e0_x_two_j215_i1  8.0392e-006
e0_x_two_j215_i2  0.44525
e0_x_two_j215_i3  0.55464
e0_x_two_j216_i1  1.3953e-005
e0_x_two_j216_i2  0.43175
e0_x_two_j216_i3  0.56824
e0_x_two_j217_i1  7.6735e-006
e0_x_two_j217_i2  0.42334
e0_x_two_j217_i3  0.57657
e0_x_two_j218_i1  1.0475e-005
e0_x_two_j218_i2  0.41744
e0_x_two_j218_i3  0.58251
e0_x_two_j219_i1  -4.7198e-008
e0_x_two_j219_i2  0.41358
```

```
e0_x_three_j31_i3   0.056609
e0_x_three_j310_i1  0.00017946
e0_x_three_j310_i2  0.94586
e0_x_three_j310_i3  0.053606
e0_x_three_j311_i1  0.00017907
e0_x_three_j311_i2  0.94585
e0_x_three_j311_i3  0.053616
e0_x_three_j312_i1  0.00016647
e0_x_three_j312_i2  0.94552
e0_x_three_j312_i3  0.054035
e0_x_three_j313_i1  0.00016557
e0_x_three_j313_i2  0.94549
e0_x_three_j313_i3  0.054059
e0_x_three_j314_i1  0.00016411
e0_x_three_j314_i2  0.94543
e0_x_three_j314_i3  0.05412
e0_x_three_j315_i1  0.00014653
e0_x_three_j315_i2  0.94489
e0_x_three_j315_i3  0.054715
e0_x_three_j316_i1  0.00010647
e0_x_three_j316_i2  0.94347
e0_x_three_j316_i3  0.056224
e0_x_three_j317_i1  0.00012603
e0_x_three_j317_i2  0.93435
e0_x_three_j317_i3  0.065315
e0_x_three_j318_i1  1.8238e-005
e0_x_three_j318_i2  0.91057
e0_x_three_j318_i3  0.089414
e0_x_three_j319_i1  2.6682e-005
e0_x_three_j319_i2  0.836
```

```
e0_x_four_j40_i3   0.90455
e0_x_four_j41_i1  -0.0004577
e0_x_four_j41_i2  0.41
e0_x_four_j41_i3  0.59339
e0_x_four_j410_i1  7.8742e-005
e0_x_four_j410_i2  0.0031165
e0_x_four_j410_i3  0.99568
e0_x_four_j411_i1  0.00010154
e0_x_four_j411_i2  0.0023024
e0_x_four_j411_i3  0.99635
e0_x_four_j412_i1  0.00011517
e0_x_four_j412_i2  0.0018772
e0_x_four_j412_i3  0.9967
e0_x_four_j413_i1  0.00012368
e0_x_four_j413_i2  0.0016499
e0_x_four_j413_i3  0.99688
e0_x_four_j414_i1  0.00012848
e0_x_four_j414_i2  0.0015293
e0_x_four_j414_i3  0.99698
e0_x_four_j415_i1  0.00013107
e0_x_four_j415_i2  0.0014656
e0_x_four_j415_i3  0.99704
e0_x_four_j416_i1  0.00013243
e0_x_four_j416_i2  0.0014312
e0_x_four_j416_i3  0.99707
e0_x_four_j417_i1  0.00013312
e0_x_four_j417_i2  0.0014113
e0_x_four_j417_i3  0.9971
e0_x_four_j418_i1  0.0001334
e0_x_four_j418_i2  0.0013959
```

Fig. 14: Liquid composition convergence results in Matlab (for every section)

Table 2: Comparison of the converged results in Matlab with Aspen Plus steady state simulation

		Aspen Plus			Matlab		
Quantity	Units	Top	Middle	Bottom	Top	Middle	Bottom
x_{C10}		1	0.00200	0	0.99308	0.00232	0.00303
x_{C14}		0	0.94702	0	0.00289	0.93997	0.00304
x_{C16}		0	0.05098	1	0.00288	0.05488	0.99412
Temp(K)		441	481	502	440	484	503

Software Comparison:

Generally, modelling tools for modelling of chemical processes can be categorized into two groups. The first group consists of readily made models with preprogramed equation systems and appropriate numerical solution algorithms. Also known as the sequential modelling approach such as Aspen Plus, Aspen HYSYS, and CHEMCAD, are some examples of software belonging to this group. Using this softwares for modelling of chemical processes can be done easily, however, it lacks in the transparency of equations involved(Stutzman *et al*., 1982). Another software may be needed to build the equations model before embedding it into those software environments. One such example is Aspen custom modeler (ACM). The second group or the equation oriented modelling provides a modelling environment based on their own programming language. The users are free to define their own equation systems by writing their own code using a specifically defined programming language. Moreover, these tools are suitable for the creation of customized models. Some examples of these tools are gProms, Aspen Custom Modeler (ACM), GAMS and MATLAB (Kuntsche *et al*., 2011b). Table 3 shows the comparison between MOSAIC, modelling tools based on the programming language (gProms, ACM, GAMS, MATLAB, C++, and Fortran), and sequential modelling approach (Aspen plus and Aspen HYSYS). Table 3 can be used as a guideline for choosing MOSAIC for any modelling and simulation work.

Table 3: Comparison of MOSAIC with other modelling tools which based on programming language, and Aspen technology.

	MOSAIC	gProms, ACM, GAMS, MATLAB, C++, and Fortran	Aspen plus, Aspen hysys	Notes
Modelling at documentation level	Available	-	-	Modelling by using MOSAIC can be done at the documentation level. Since the equations are written in LaTeX documentary language, it has similar readability as the documentation level. In addition, coding is not required for modelling using MOSAIC.

Reuse of model elements	Available	Partially available	-	The reuse of model elements by MOSAIC is more systematic and organized. The users can either reuse the notation, equations, functions, and variables settings easily.
Code generation	Available	Not complete	-	Code generation by MOSAIC is a lot more complete. MOSAIC allows users to generate the code and run their models in many different environments.
Centralized internet database capability	Available	-	-	MOSAIC allows users to share their work over the internet more easily. The shared work can be viewed or written by the person that users shared to.
Degree of freedom analysis	Available	-	-	The degree of freedom analysis can be done automatically by MOSAIC. In order to generate code for evaluations, the degree of freedom must be zero. Hence, it is necessary for the model to have correct equations in an equation system and all errors must be corrected.
Error identification	Excellent	Difficult	-	Since models in MOSAIC are written in LaTeX documentary language, it has high readability. Hence, users can identify errors more easily if they are making mistakes while keying in modelling equations. In addition, coding is not required by MOSAIC, hence it results in fewer errors and less effort.
Language	Documentary	Programing	-	MOSAIC is using LaTeX documentary language in writing of modelling equations. LaTeX has high readability, unlike programming language, it is difficult to read and understand the coding.
Readability	Excellent	Poor	-	LaTeX documentary language has much higher readability than programming languages since MOSAIC use two-dimensional symbolic language.
Difficulty	Medium	Hard	Easy	Although without knowledge of coding in modelling, MOSAIC still allows users to do modelling without a doubt. The stages of modelling using MOSAIC are creating of notation, creating of equations, creating of functions, creating of equation system, creating of parameter object and creating of evaluation object. The most difficult part will be creating of functions, however, it can overcome easily once users know how it works.
Transparency of model	Excellent	Excellent	Poor	All equations involved in modelling are known for MOSAIC. Besides that, given values of variables can also be determined.
Building of customized model	Capable	Capable	Not capable	MOSAIC is similar to software like Matlab which is designed to build the customized model.

Conclusion:

This work presents an equation oriented modelling of DWC using MOSAIC. In order to obtain a good convergence and reliable results in modeling, it is important to have good guess initial values of iteration variables. Hence, based on the case study, the developed model simulation in MOSAIC agrees with data taken for the same process in Aspen Plus as an initial iteration values in MOSAIC. The results show that MOSAIC provide a good functionality in code generator that can translate the specified models into program code for Matlab. Using MOSAIC, the modelling approach does not require any written code as such it is much easier to learn and less prone to a programming error. In addition, the model formulation has the same readability as the documentation level. Besides that, reuse of model elements can be done effectively thus reduce the efforts of modelling. This work also compares the features between modelling in MOSAIC and programming language, as well as simulation work. Such comparison could help researchers to decide in using MOSAIC for any modelling work.

ACKNOWLEDGEMENT

This work is supported by Malaysia Ministry of Education under grant no. RDU130601 and RDU140105.

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