ProSim

BATCHREACTOR APPLICATION EXAMPLE

FOOD INDUSTRY

SIMULATION OF BATCH TOMATO SAUCE OXIDATION

EXAMPLE PURPOSE
The main interest of this example is to show how user can very simply describe his own kinetics models using the advanced mode available in Simulis Reactions, the chemical reactions server used in BatchReactor software. This food processing example deals with reactions that some components of the tomato sauce, such as ascorbic acid, chlorogenic acid and β-carotene, suffer during the production of this product. The studied reactions involve the oxidation and degradation of the first cited compound, the oxidation of the second one and the isomerization of the third one. The oxygen transfer which influences the oxidation reactions is represented by a chemical reaction in which the reagent is the oxygen in gas phase and the product is the dissolved oxygen. The mathematical modeling of the reaction mechanisms (Arrhenius law with different parameters sets depending on the temperature domain and oxygen transfer law) uses specific equations which are not available in standard chemical reaction libraries such as Simulis Reactions.

ACCESS	☑ Free-Internet	☐ Restricted to ProSim clients	☐ Restricted	☐ Confidential

CORRESPONDING BATCHREACTOR FILES	*BATCHREA_E02_EN - Tomato sauce Run 050C.pbpr* *BATCHREA_E02_EN - Tomato sauce Run 070C .pbpr* *BATCHREA_E02_EN - Tomato sauce Run 095C.pbpr* *BATCHREA_E02_EN - Tomato sauce Run 105C.pbpr*

Reader is reminded that this use case is only an example and should not be used for other purposes. Although this example is based on actual case it may not be considered as typical nor are the data used always the most accurate available. ProSim shall have no responsibility or liability for damages arising out of or related to the use of the results of calculations based on this example.

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1. INTRODUCTION

This example involves the study of the reactions that occur during the production of tomato sauce during the transformation of fresh tomatoes into concentrated sauce.

Five main reactions are studied: the ascorbic acid oxidation and degradation, the chlorogenic acid oxidation, the β-carotene isomerization and the oxygen transfer. Regarding the oxidations, the ascorbic acid reacts with oxygen to give dehydroascorbic acid and hydrogen peroxide, while chlorogenic acid reacts with oxygen to give a quinone and again, hydrogen peroxide. It is thus observed that these two reactions are limited by the oxygen transfer to the liquid phase where they take place. This transfer has to be taken into account so the model representing this process can be more accurate. In the isomerization, the reagent is the E-carotene (trans-isomer), which reacts to form Z-carotene (cis-isomer). Finally, for the degradation of the ascorbic acid it is considered that one molecule of this substance gives one molecule of degraded ascorbic acid.

All reactions are considered to follow the Arrhenius law and the values for the activation energy and the pre-exponential factor were taken from [BRA12]. Nevertheless, parameters of these Arrehnius laws depend on the temperature range.

2. REACTION MECHANISM

The reactions taken into account during the transformation of fresh tomatoes into concentrated sauce are the following ones:

- ✓ Chlorogenic acid oxidation:

$$Chlorogenic\ acid + Oxygen \rightarrow Chlorogenic\ acid\ quinone + Hydrogen\ peroxide$$

Namely,

$$C_{16}H_{18}O_9 + O_2 \rightarrow C_{16}H_{16}O_9 + H_2O_2 \quad \text{(R1)}$$

- ✓ Ascorbic acid oxidation:

$$Ascorbic\ acid + Oxygen \rightarrow Dehydroascorbic\ acid + Hydrogen\ peroxide$$

Namely,

$$C_6H_8O_6 + O_2 \rightarrow C_6H_6O_6 + H_2O_2 \quad \text{(R2)}$$

- ✓ Ascorbic acid thermal degradation:

$$Ascorbic\ acid \rightarrow Degraded\ ascorbic\ acid$$

Namely,

$$C_6H_8O_6 \rightarrow C_6H_8O_{6(degraded)} \quad \text{(R3)}$$

- ✓ β-carotene isomerization:

$$E-carotene \rightarrow Z-carotene$$

Namely,

$$C_{40}H_{56(trans)} \rightarrow C_{40}H_{56(cis)} \quad \text{(R4)}$$

- ✓ Oxygen transfer:

$$gas\ oxygen \rightarrow dissolved\ oxygen$$

Namely,

$$O_{2(gas\ phase)} \rightarrow O_{2(liquid\ phase)} \quad \text{(R5)}$$

3. COMPONENTS

Components which are taken into account in the simulation are:

Name	CAS number
Oxygen (gas phase) (*)	
Oxygen (liquid phase) (*)	
Water(*)	7732-18-5
Hydrogen peroxide(*)	7722-84-1
Ascorbic acid(*)	50-81-7
Degraded ascorbic acid(*)	
Dehydroascorbic acid	
Chlorogenic acid	
Chlorogenic acid quinone	
E-carotene	
Z-carotene	
Dry matter	

Compounds with an asterisk are taken from the standard database of Simulis Thermodynamics, thermodynamics server used in BatchReactor. The thermophysical parameters stored in this database are the DIPPR recommended values [ROW11].

The two “types” of oxygen are cloned from the oxygen compound of this database. Their vapor pressure correlations are changed to insure that the “liquid oxygen” is non volatile and that the “gas oxygen” is non-condensable. Furthermore, both CAS numbers were changed to arbitrary numbers.

$$Ln\left(P^{0}\right)=A+\frac{B}{T}+CLn\left(T\right)+DT^{E} \qquad \left(Equation\ 101\right)$$

Coefficient	“Gas oxygen”	“Liquid oxygen”
A	30	-30
B, C, D, E	0	0

The “degraded ascorbic acid” compound is a clone of the ascorbic acid compound. Only the CAS number has been changed (arbitrary number).

The other compounds (dehydroascorbic acid, chlorogenic acid, chlorogenic acid quinone, E-carotene, Z-carotene and dry matter) were created by the function “Add a new compound” of Simulis Thermodynamics. The properties which are specified are the following ones:

- ✓ CAS number : Arbitrary number
- ✓ Chemical formula : From literature
- ✓ Molecular weight : From literature
- ✓ Enthalpy of formation for ideal gas at 25°C : 0 J/mol
- ✓ Vapor and liquid mass specific heat : Same as water

- ✓ Vapor pressure : Parameters chosen to avoid the vaporization

$$Ln\left(P^0\right) = -30 \qquad (Equation\ 101)$$

- ✓ Vaporization enthalpy : 0 J/mol
- ✓ Liquid density : Same as water

The dry matter compound was created because all of the experimental data is based on the dry matter quantity in the system. A molecular weight of 1 g/mol is adopted. This compound is considered as an insoluble solid.

4. THERMODYNAMIC MODEL

Reactions occurred at temperature up to 105°C and atmospheric pressure, so the gas phase was assumed to follow the Perfect Gas law.

The liquid phase contains an insoluble solid, the dry matter. This solid has been represented as a non-volatile liquid (see § 3). It should be excluded from the liquid phase for the vapor-liquid equilibrium. If not, it modifies the real compositions of the liquid phase and so the vapor-liquid equilibrium constant of water, the volatile component. Thus, the “Solids excluded from liquid phase” model has been selected to calculate the liquid fugacity.

5. REACTION MATHEMATICAL MODEL

[BRA12] developed a mathematical model for the reactions which occure during the production of tomato sauce (transformation of fresh tomatoes into concentrated sauce).

- ✓ Rate of the chlorogenic acid oxidation:

$$r_{ACHL} = k_{ACHL,0} \exp\left(\frac{-Ea_{ACHL}}{RT}\right)[ACHL] \quad \text{(R1)}$$

- ✓ Rate of the ascorbic acid oxidation:

$$r_{AASC} = k_{AASC,0} \exp\left(\frac{-Ea_{AASC}}{RT}\right)[AASC] \quad \text{(R2)}$$

- ✓ Rate of the ascorbic acid degradation:

$$r_{AASC(degrad)} = k_{AASC(degrad),0} \exp\left(\frac{-A_{AASC(degrad)}}{T}\right)[AASC] \quad \text{(R3)}$$

- ✓ Rate of β-carotene isomerization:

$$r_{Caro} = k_{Caro,0} \exp\left(\frac{-Ea_{Caro}}{RT}\right)[E_{Carotene}] \quad \text{(R4)}$$

- ✓ Rate of oxygen transfer:

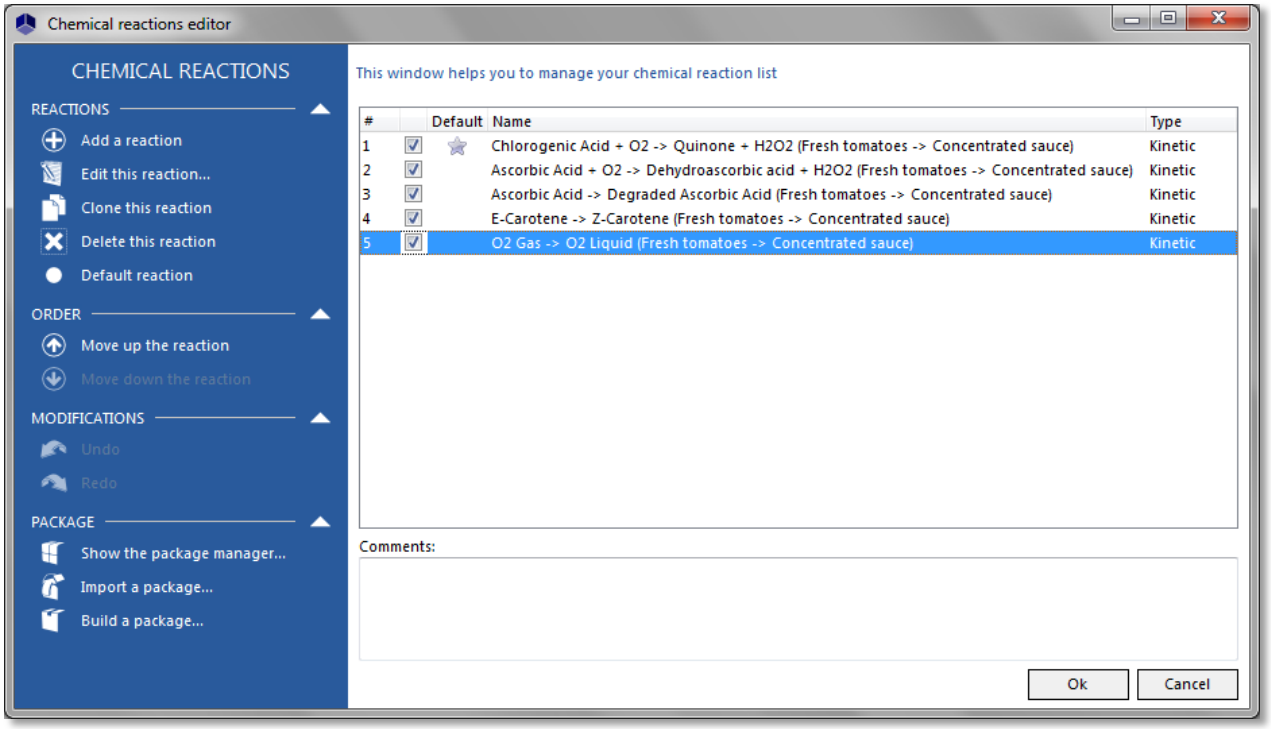
$$r_{O_2} = k_L a_{O_2,0} \exp\left(\frac{-A_{O_2}}{T}\right)\left([O_{2(saturation)}] - [O_{2(dissous)}]\right) \quad \text{(R5)}$$

All parameters taken from [BRA12] are presented in the following table. Outside the different temperature ranges, it is assumed that the corresponding reactions doesn't occurred, i.e. $r_i = 0$.

Compound	Temperature range	Parameters
Chlorogenic acid (ACHL)	25°C – 95°C	$k_{ACHL,0} = 5180\,\text{min}^{-1}$ $Ea_{ACHL} = 35100\,J/mol$
Ascorbic acid (AASC)	25°C – 95°C	$k_{AASC,0} = 12300\,\text{min}^{-1}$ $Ea_{AASC} = 37400\,J/mol$
	25°C – 125°C	$k_{AASC(degrad),0} = 1.75x10^6\,\text{min}^{-1}$ $A_{AASC(degrad)} = 7480K$
β-Carotene (Caro)	95°C – 125°C	$k_{Caro,0} = 2070\,\text{min}^{-1}$ $Ea_{Caro} = 39300\,J/mol$
Oxygen transfer	25°C – 95°C	$k_{Oxygen,0} = 1.73x10^6\,\text{min}^{-1}$ $A_{Oxygen} = 5080K$

6. REACTION MODEL IMPLEMENTATION USING SIMULIS REACTIONS

The five reactions presented in the paragraphs 2 and 5 were described in Simulis Reactions, as shown in the next screen shot.

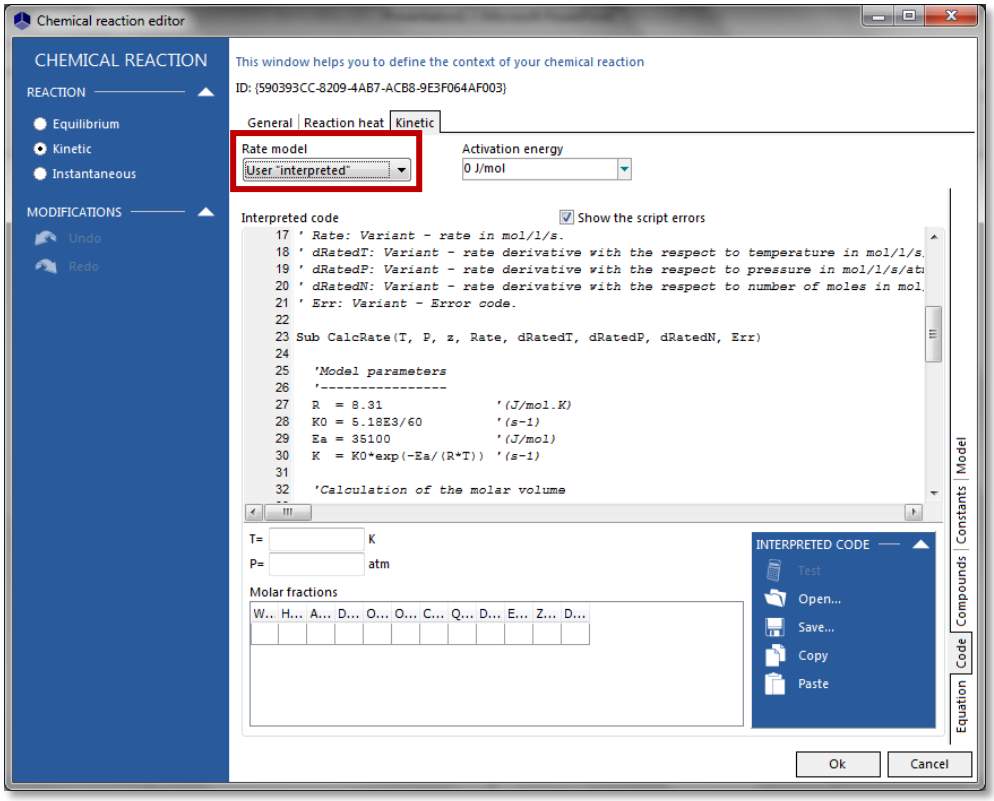


As the kinetics parameters of the reactions changes according to the range of temperature, user “interpreted” kinetic rate model was used to implement mathematical models presented by [BRA12] for the five reactions, as shown on the next screenshot. Thanks to this functionality of Simulis Reactions, user can write his own code for kinetic model using VBScript (Microsoft Visual Basic Scripting Edition), which is an interpreted language: it doesn’t require compilation before being executed and it requires the computer that has to run it has an interpreter (i.e. a program that can understand the whole instructions, e.g. *wscript.exe* in Windows environment). For more information about VBScript language, user can refer to:

http://msdn.microsoft.com/en-us/library/t0aew7h6(v=vs.84).aspx

http://en.wikipedia.org/wiki/VBScript

All reactions take place in the liquid phase. The heat of reaction of each reaction is assumed to be 0.



The VBS code for the (R1) reaction is the following one:

```
' CHECK PROCEDURE

Function CheckRate

  CheckRate = True

End Function



' CALCULATION PROCEDURE

' --- Data ---

' T: Variant - Temperature (K).

' P: Variant - Pressure (atm).

' z: Variant - Molar fractions.

' --- Results ---

' Rate: Variant - rate in mol/l/s.

' dRatedT: Variant - rate derivative with the respect to temperature in mol/l/s/K.

' dRatedP: Variant - rate derivative with the respect to pressure in mol/l/s/atm.

' dRatedN: Variant - rate derivative with the respect to number of moles in mol/l/s.

' Err: Variant - Error code.

Sub CalcRate(T, P, z, Rate, dRatedT, dRatedP, dRatedN, Err)

  'Model parameters

  R  = 8.31              '(J/mol.K)

  K0 = 5.18E3/60         '(s-1)

  Ea = 35100             '(J/mol)
```



```
  K  = K0*exp(-Ea/(R*T)) '(s-1)

  'Calculation of the molar volume

  Vml=ThermoCalculator.PCalcVml(T,P,z)

  'Units conversion

  Set Repository = CreateObject("CverStarDustRepository.StarDust_CVER_Repository")

  Set Quantity   = Repository.QuantityByName("Molar volume")

  Vml            =  Quantity.Convert(Vml,"cm3/mol","l/mol")

  Set MwQty      = Repository.QuantityByName("Molar mass")

  'Calculation of the concentrations

  CASN_ChloroAcid = "55010-02-1"

  For i=1 To ThermoCalculator.Compounds.Count

    With ThermoCalculator.Compounds.Items(i-1)

      If (.CasRegistryNumber = CASN_ChloroAcid) Then

          ipos_ChloroAcid = i-1

          Mw_ChloroAcid   = MwQty.Convert(.Mw.Value,.Mw.UnitName,"g/mol")

          C_ChloroAcid    = z(ipos_ChloroAcid)*Mw_ChloroAcid/Vml

      End If

    End With

  Next

  'Calculation of the reaction rate

  If (T >= 298.1 And T <= 368.2) Then 'Temperature between 25°C and 95°C

      Rate = K*C_ChloroAcid           '(g/L.s)

      Rate = Rate/Mw_ChloroAcid       '(mol/L.s)

  Else

      Rate = 0

  End If

End Sub
```

The VBS code for the (R2) reaction is the following one:

```
' CHECK PROCEDURE

Function CheckRate

  CheckRate = True

End Function


' CALCULATION PROCEDURE

' --- Data ---

' T: Variant - Temperature (K).

' P: Variant - Pressure (atm).

' z: Variant - Molar fractions.

' --- Results ---
```



```
' Rate: Variant - rate in mol/l/s.

' dRatedT: Variant - rate derivative with the respect to temperature in mol/l/s/K.

' dRatedP: Variant - rate derivative with the respect to pressure in mol/l/s/atm.

' dRatedN: Variant - rate derivative with the respect to number of moles in mol/l/s.

' Err: Variant - Error code.

Sub CalcRate(T, P, z, Rate, dRatedT, dRatedP, dRatedN, Err)

  'Model parameters

  R  = 8.31              '(J/mol.K)

  K0 = 12.3E3/60         '(s-1.100g/mg)

  Ea = 37400             '(J/mol)

  K  = K0*exp(-Ea/(R*T)) '(s-1)

  'Calculation of the concentration of oxygen at saturation and K with the correct unit

  C_SaturatedOxygen = -2.487635154965E-08*T^3+0.0000247773387665511*T^2-0.00830230726171837*T+0.940377326855335 '(g/l)

  C_SaturatedOxygen = C_SaturatedOxygen*100                                                                    '(mg/100g)

  K                 = K*C_SaturatedOxygen                                                                        '(s-1)

  'Calculation of the molar volume

  Vml=ThermoCalculator.PCalcVml(T,P,z)

  'Units conversion

  Set Repository = CreateObject("CverStarDustRepository.StarDust_CVER_Repository")

  Set Quantity   = Repository.QuantityByName("Molar volume")

  Vml            =  Quantity.Convert(Vml,"cm3/mol","l/mol")

  Set MwQty      = Repository.QuantityByName("Molar mass")

  'Calculation of the concentrations

  CASN_AscorbicAcid = "50-81-7"

  For i=1 To ThermoCalculator.Compounds.Count

    With ThermoCalculator.Compounds.Items(i-1)

      If (.CasRegistryNumber = CASN_AscorbicAcid) Then

          ipos_AscorbicAcid = i-1

          Mw_AscorbicAcid   = MwQty.Convert(.Mw.Value,.Mw.UnitName,"g/mol")

          C_AscorbicAcid    = z(ipos_AscorbicAcid)*Mw_AscorbicAcid/Vml

      End If

    End With

  Next

  'Calculation of the reaction rate

  If (T >= 298.1 And T <= 368.2) Then 'Temperature between 25°C and 95°C

      Rate = K*C_AscorbicAcid        '(g/L.s)

      Rate = Rate/Mw_AscorbicAcid    '(mol/L.s)

  Else

      Rate = 0

  End If

End Sub
```


The VBS code for the (R3) reaction is the following one:

```
' CHECK PROCEDURE

Function CheckRate

  CheckRate = True

End Function


' CALCULATION PROCEDURE

' --- Data ---

' T: Variant - Temperature (K).

' P: Variant - Pressure (atm).

' z: Variant - Molar fractions.

' --- Results ---

' Rate: Variant - rate in mol/l/s.

' dRatedT: Variant - rate derivative with the respect to temperature in mol/l/s/K.

' dRatedP: Variant - rate derivative with the respect to pressure in mol/l/s/atm.

' dRatedN: Variant - rate derivative with the respect to number of moles in mol/l/s.

' Err: Variant - Error code.

Sub CalcRate(T, P, z, Rate, dRatedT, dRatedP, dRatedN, Err)

  'Model parameters

  R  = 8.31        '(J/mol.K)

  K0 = 1.75E6/60   '(s-1)

  A  = 7.48E3      '(K)

  K = K0*exp(-A/T) '(s-1)

  'Calculation of the molar volume

  Vml=ThermoCalculator.PCalcVml(T,P,z)

  'Units conversion

  Set Repository = CreateObject("CverStarDustRepository.StarDust_CVER_Repository")

  Set Quantity   = Repository.QuantityByName("Molar volume")

  Vml            =  Quantity.Convert(Vml,"cm3/mol","l/mol")

  Set MwQty      = Repository.QuantityByName("Molar mass")

  'Calculation of the concentrations

  CASN_AscorbicAcid = "50-81-7"

  For i=1 To ThermoCalculator.Compounds.Count

    With ThermoCalculator.Compounds.Items(i-1)

      If (.CasRegistryNumber = CASN_AscorbicAcid) Then

          ipos_AscorbicAcid = i-1

          Mw_AscorbicAcid   = MwQty.Convert(.Mw.Value,.Mw.UnitName,"g/mol")

          C_AscorbicAcid    = z(ipos_AscorbicAcid)*Mw_AscorbicAcid/Vml

      End If

    End With

  Next
```



```
  'Calculation of the reaction rate

  If (T >= 298.1 And T <= 398.2) Then 'Temperature between 25°C and 125°C

      Rate = K*C_AscorbicAcid        '(g/L.s)

      Rate = Rate/Mw_AscorbicAcid    '(mol/L.s)

  Else

      Rate = 0

  End If

End Sub
```

The VBS code for the (R4) reaction is the following one:

```
' CHECK PROCEDURE

Function CheckRate

  CheckRate = True

End Function


' CALCULATION PROCEDURE

' --- Data ---

' T: Variant - Temperature (K).

' P: Variant - Pressure (atm).

' z: Variant - Molar fractions.

' --- Results ---

' Rate: Variant - rate in mol/l/s.

' dRatedT: Variant - rate derivative with the respect to temperature in mol/l/s/K.

' dRatedP: Variant - rate derivative with the respect to pressure in mol/l/s/atm.

' dRatedN: Variant - rate derivative with the respect to number of moles in mol/l/s.

' Err: Variant - Error code.

Sub CalcRate(T, P, z, Rate, dRatedT, dRatedP, dRatedN, Err)

  'Model parameters

  R  = 8.31              '(J/mol.K)

  K0 = 2.07E3/60         '(s-1)

  Ea = 39300             '(J/mol)

  K  = K0*exp(-Ea/(R*T)) '(s-1)

  'Calculation of the molar volume

  Vml=ThermoCalculator.PCalcVml(T,P,z)

  'Units conversion

  Set Repository = CreateObject("CverStarDustRepository.StarDust_CVER_Repository")

  Set Quantity   = Repository.QuantityByName("Molar volume")

  Vml            =  Quantity.Convert(Vml,"cm3/mol","l/mol")

  Set MwQty      = Repository.QuantityByName("Molar mass")

  'Calculation of the concentrations
```



```
  CASN_ECarotene = "55310-01-5"
  For i=1 To ThermoCalculator.Compounds.Count
    With ThermoCalculator.Compounds.Items(i-1)
      If (.CasRegistryNumber = CASN_ECarotene) Then
          ipos_ECarotene = i-1
          Mw_ECarotene   = MwQty.Convert(.Mw.Value,.Mw.UnitName,"g/mol")
          C_ECarotene    = z(ipos_ECarotene)*Mw_ECarotene/Vml
      End If
    End With
  Next
  'Calculation of the reaction rate
  If (T >= 368.1 And T <= 398.2) Then 'Temperature between 95°C and 125°C
      Rate = K*C_ECarotene            '(g/L.s)
      Rate = Rate/Mw_ECarotene        '(mol/L.s)
  Else
      Rate = 0
  End If
End Sub
```

The VBS code for the (R5) reaction is the following one:

```
' CHECK PROCEDURE
Function CheckRate
  CheckRate = True
End Function


' CALCULATION PROCEDURE
' --- Data ---
' T: Variant - Temperature (K).
' P: Variant - Pressure (atm).
' z: Variant - Molar fractions.
 --- Results ---
' Rate: Variant - rate in mol/l/s.
' dRatedT: Variant - rate derivative with the respect to temperature in mol/l/s/K.
' dRatedP: Variant - rate derivative with the respect to pressure in mol/l/s/atm.
' dRatedN: Variant - rate derivative with the respect to number of moles in mol/l/s.
' Err: Variant - Error code.
Sub CalcRate(T, P, z, Rate, dRatedT, dRatedP, dRatedN, Err)
  'Model parameters (Temperature between 50 and 80°C)
  Kla0 = 1.73E6/60      '(s-1)
  A    = 5.08E3         '(K)
```



```
  Kla  = Kla0*exp(-A/T) '(s-1)

  'Calculation of the molar volume

  Vml=ThermoCalculator.PCalcVml(T,P,z)

  'Units conversion

  Set Repository = CreateObject("CverStarDustRepository.StarDust_CVER_Repository")

  Set Quantity   = Repository.QuantityByName("Molar volume")

  Vml            =  Quantity.Convert(Vml,"cm3/mol","l/mol")

  Set MwQty      = Repository.QuantityByName("Molar mass")

  'Calculation of the concentrations

  CASN_LiquidOxygen = "55010-01-0"

  For i=1 To ThermoCalculator.Compounds.Count

    With ThermoCalculator.Compounds.Items(i-1)

      If (.CasRegistryNumber = CASN_LiquidOxygen) Then

          ipos_LiquidOxygen = i-1

          Mw_LiquidOxygen   = MwQty.Convert(.Mw.Value,.Mw.UnitName,"g/mol")

          C_LiquidOxygen    = z(ipos_LiquidOxygen)*Mw_LiquidOxygen/Vml

      End If

    End With

  Next

  'Calculation of the concentration of oxygen at saturation (g/l)

   C_SaturatedOxygen = -2.487635154965E-08*T^3+0.000024777338766551 1*T^2-0.00830230726171837*T+0.940377326855335

  'Calculation of the reaction rate

  If (T >= 298.1 And T <= 368.2) Then             'Temperature between 25°C and 95°C

    Rate = Kla*(C_SaturatedOxygen-C_LiquidOxygen) '(g/L.s)

    Rate = Rate/Mw_LiquidOxygen                   '(mol/L.s)

  Else

      Rate = 0

  End If

End Sub
```


7. SIMULATION

7.1. Process description

The characteristics of the reactor used for the concentration of fresh tomatoes are described in the table below.

Reactor	
Type	Closed vapor-liquid
Global volume (vapor + liquid)	500 l
Head space Type Adjustment variable "Pressurizing" compound	 Other Pressure Oxygen (Gas)

The initial conditions are presented in the following table. For the case T = 105°C an operating pressure of 1.3 atm was chosen to avoid water evaporation from the solution. A mass of 10 kg of dry matter is chosen and all the other compounds initial loads are calculated according to this quantity. It is assumed that the dry matter represents approximatively 5 wt.% of the initial load. Thus the water initial load was 200 kg. For the oxygen in liquid phase, the initial load is chosen according to the solubility of this compound in water [PRO15].

	Experimental conditions [BRA12]				**Simulation initial conditions**			
Temperature	50°C	70°C	95°C	105°C	50°C	70°C	95°C	105°C
Pressure	Not specified				1 atm			1.3 atm
	Experimental concentration [BRA12] (mg/100g$_{dry\ matter}$)				**Simulation initial loads**			
Water	Not specified				200 kg			
Dry matter	Not specified				10 kg			
Chlorogenic acid	8.88	Not specified			0.888 g			
Ascorbic acid	282	338	271	247	28.2 g	33.8 g	27.1 g	24.7 g
E-carotene	Not specified		4.24	Not specified	0.424 g			
Oxygen (liquid phase)	Not specified				1 g	0.6 g	0.16 g	0 g
Other compound	0				0 g			

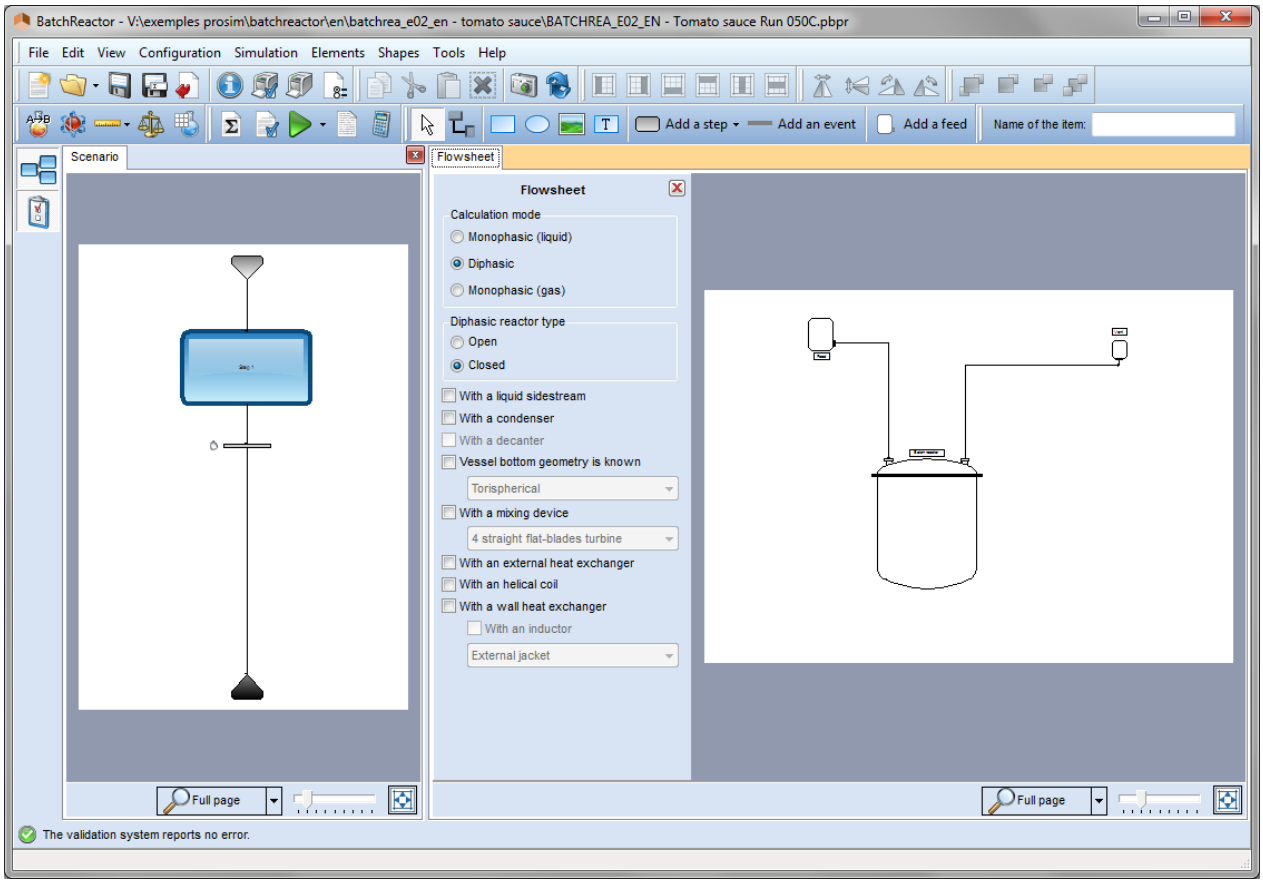
A continuous oxygen gas stream feeds the reactor in order to assure that the availability of oxygen in gas phase is not limiting. The characteristics of this stream are:

Temperature	50°C	70°C	95°C	105°C
Pressure	1 atm			1.3 atm
Total flow rate	10 kg/h			
Mole fractions				
Oxygen	1			
Other components	0			

The recipe consists in one isothermal step with the following parameters:

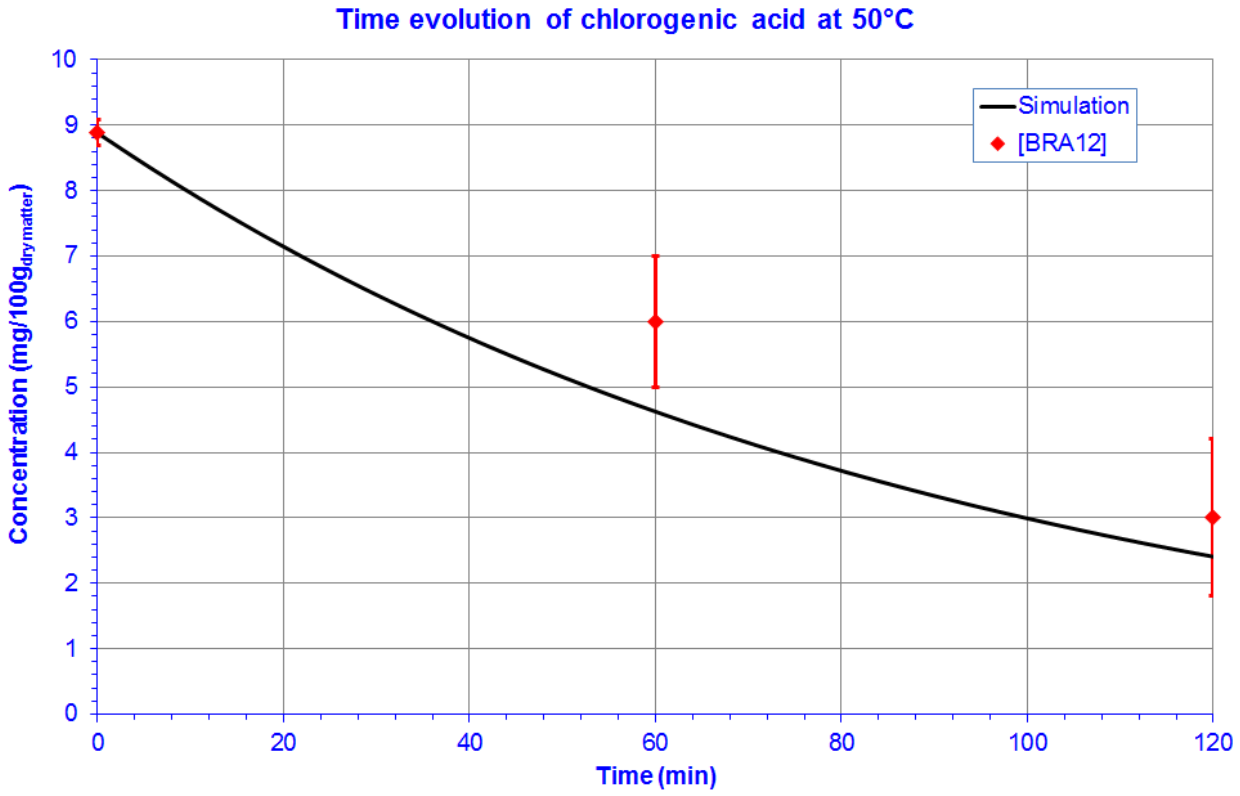
Type	Specified TR without thermal device			
Temperature	50°C	70°C	95°C	105°C
Pressure	1 atm			1.3 atm
Step duration	2 h		1 h	

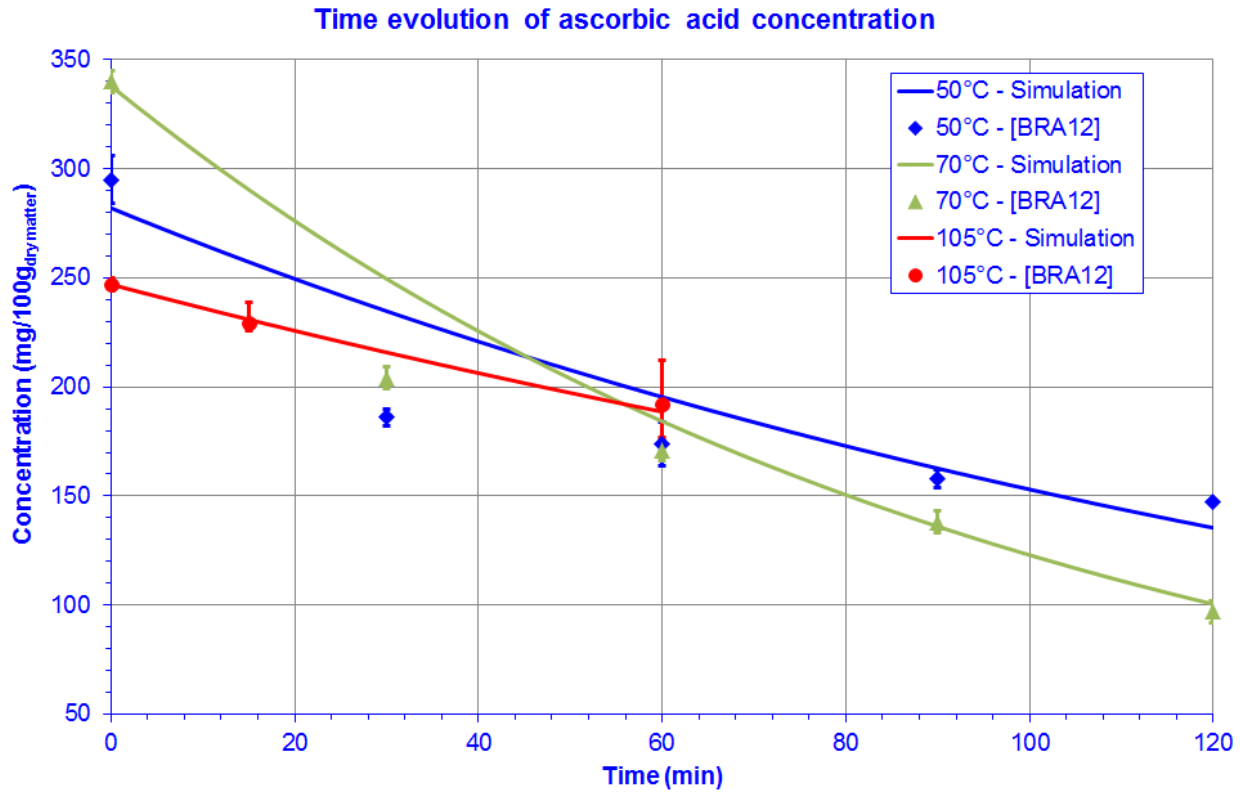
The following screen shot presents the simulation of the run at 50°C. The scenario is presented on the left part of this screen shot and the flowsheet on the right part.

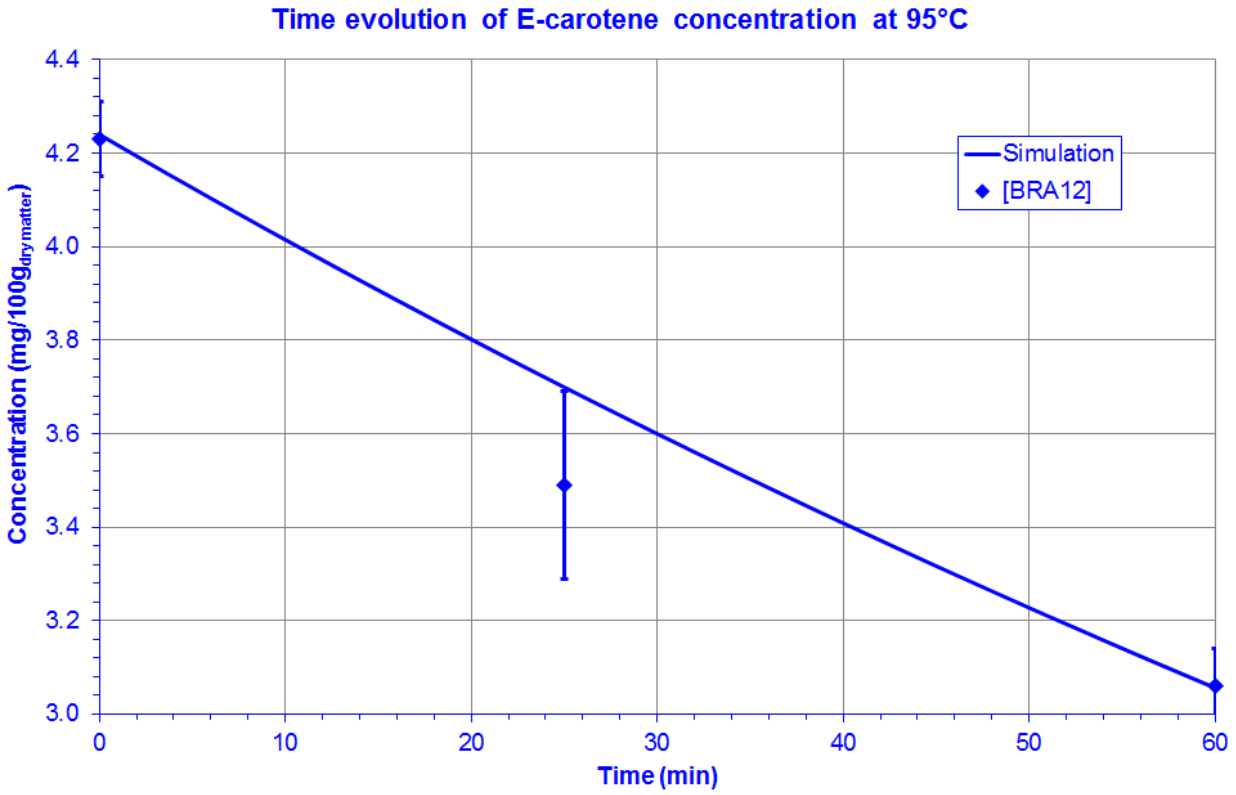


7.2. Results

Comparisons between concentration profiles obtained with BatchReactor software and information given by [BRA12] are provided on the next graph.







8. REFERENCES

[BRA12] BRANDAM C., MEYER X., ROLAND M., “Application et validation industrielle d’un modèle prédictif de la qualité nutritionnelle de produits à base de tomate au cours des procédés de fabrication”, DGAL Convention a13 PACA 05 12-1

[PRO15] http://protec.pagesperso-orange.fr/22_Solubilite_de_l'oxygene.htm (link verify in September 2015)

[ROW11] ROWLEY R.L., WILDING W.V., OSCARSON J.L., GILES N.F., “DIPPR® Data Compilation of Pure Chemical Properties”, Design Institute for Physical Properties, AIChE, New York, NY (2011)

9. NOMENCLATURE

$[AASC]$	Concentration of ascorbic acid	g/l
$[ACHL]$	Concentration of chlorogenic acid	g/l
A_i	Kinetic constant	K
Ea_i	Activation energy	J/mol
$[E_{Carotene}]$	Concentration of E-Carotene	g/l
$k_{i,0}$	Pre-exponential factor	min^{-1}
$[O_{2(dissolved)}]$	Concentration of dissolved oxygen	g/l
$[O_{2(saturation)}]$	Saturation concentration of dissolved oxygen in the operating temperature	
	(taken from the Winkler table in [PRO15]	(g/l)
R	Perfect gas constant	J/(mol.K)
r_i	Rates of the reaction	g/(l.s)
T	Temperature	K

