SUPPLEMENTARY FIGURES

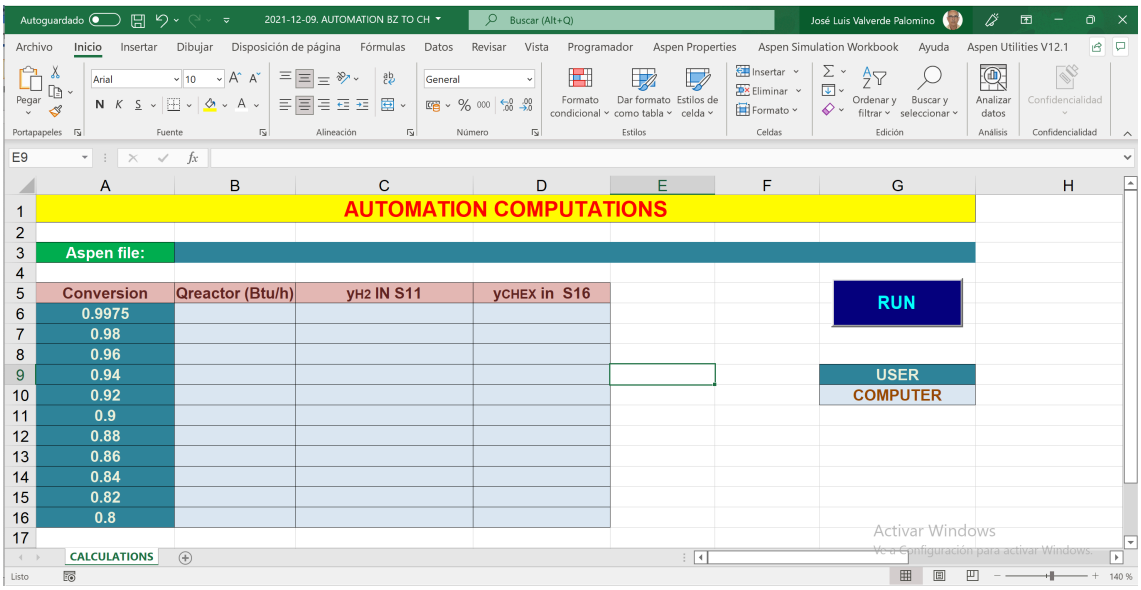


Figure S1. Sheet COMPUTATIONS in the MS EXCEL-VBA template used in Case of Study 1.

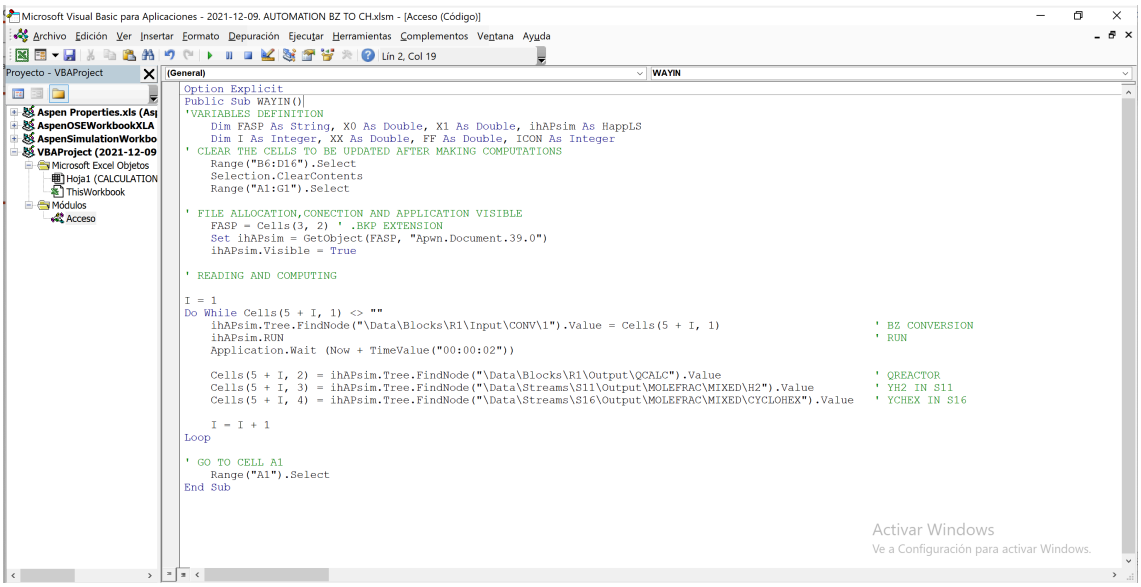


Figure S2. Definition of module Acceso used in Case of Study 1.

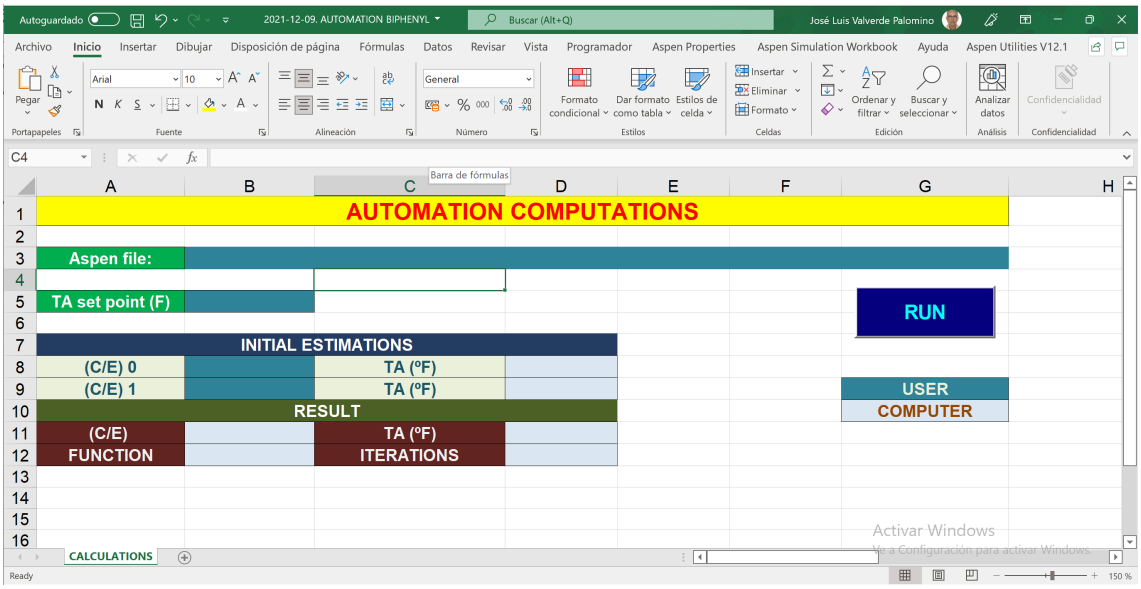


Figure S3. Sheet COMPUTATIONS in the MS EXCEL-VBA template used in Case of Study 2.

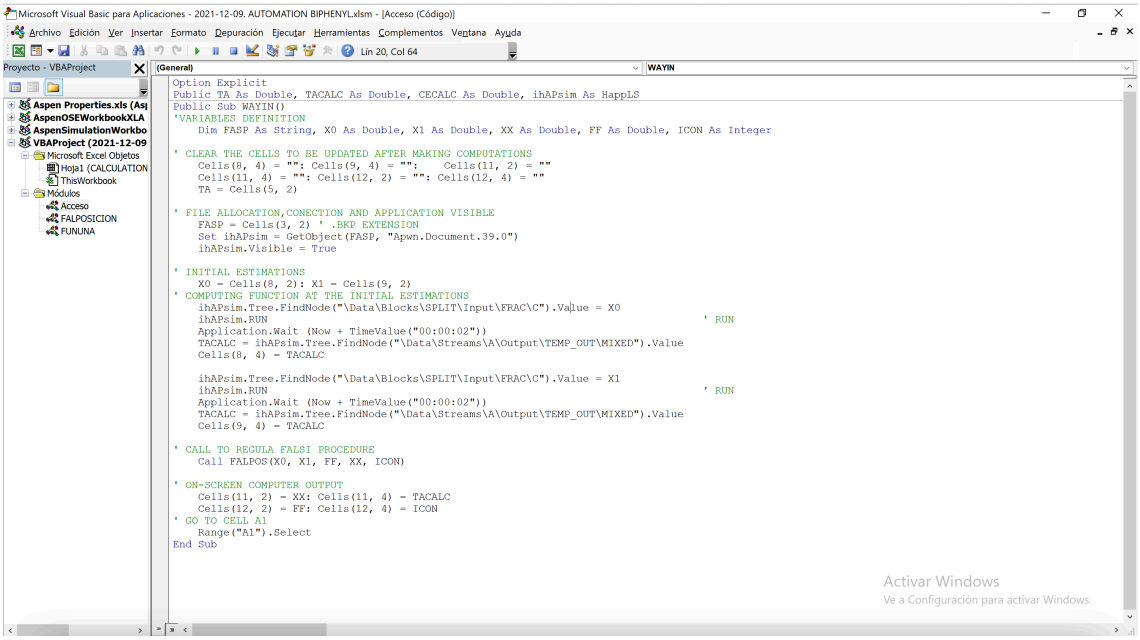


Figure S4. Definition of module Acceso used in Case of Study 2.

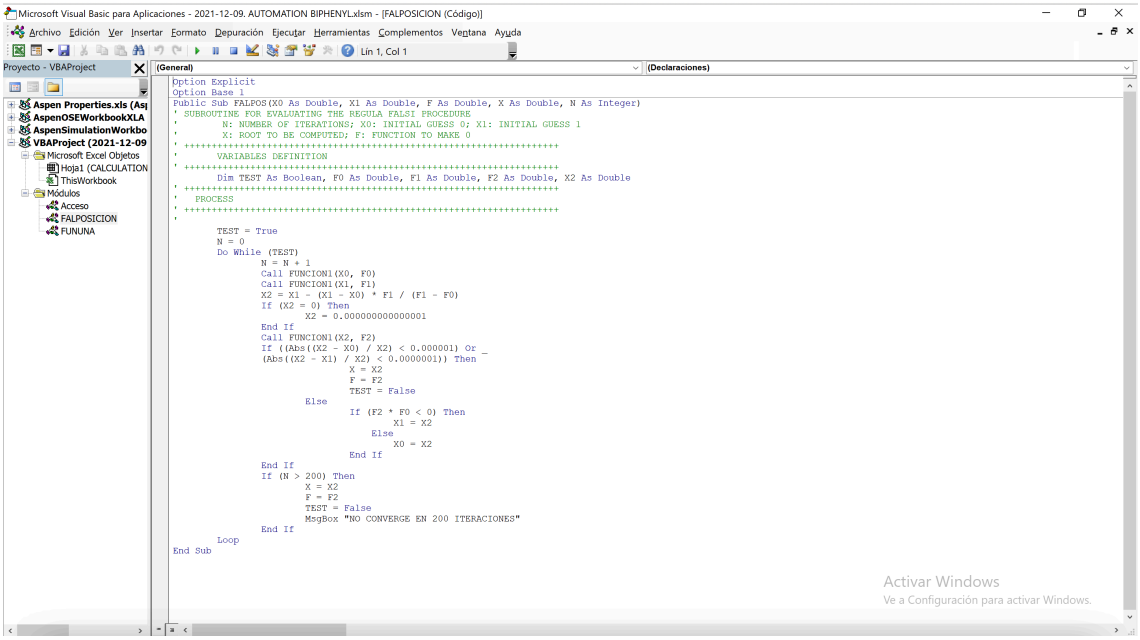


Figure S5. Definition of module FALPOSICION used in Case of Study 2.

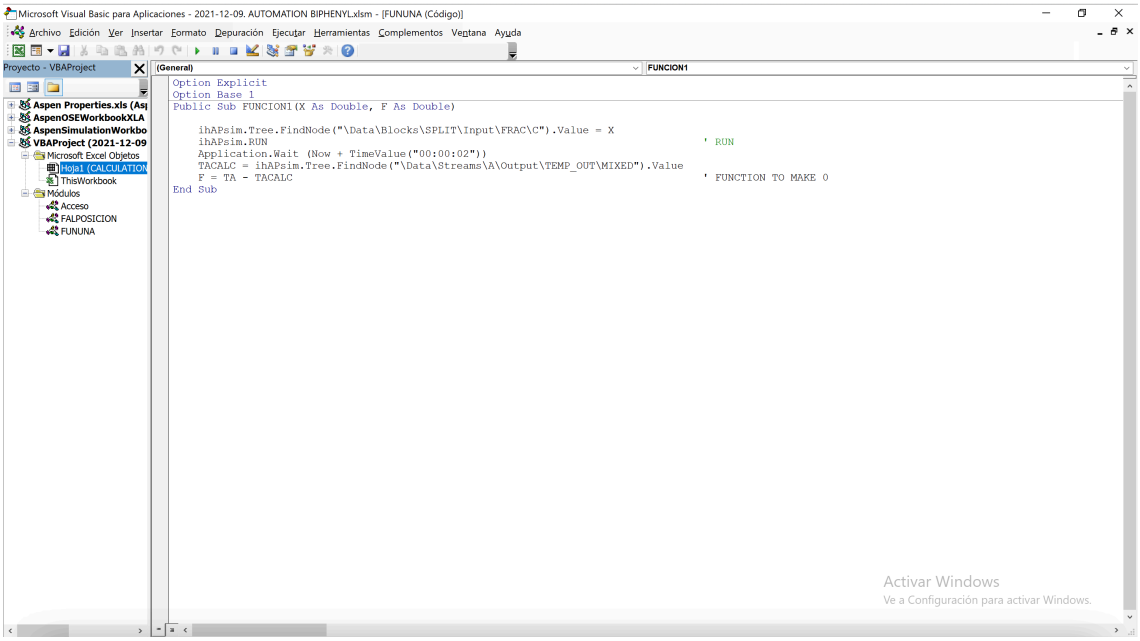


Figure S6. Definition of module FUNUNA used in Case of Study 2.

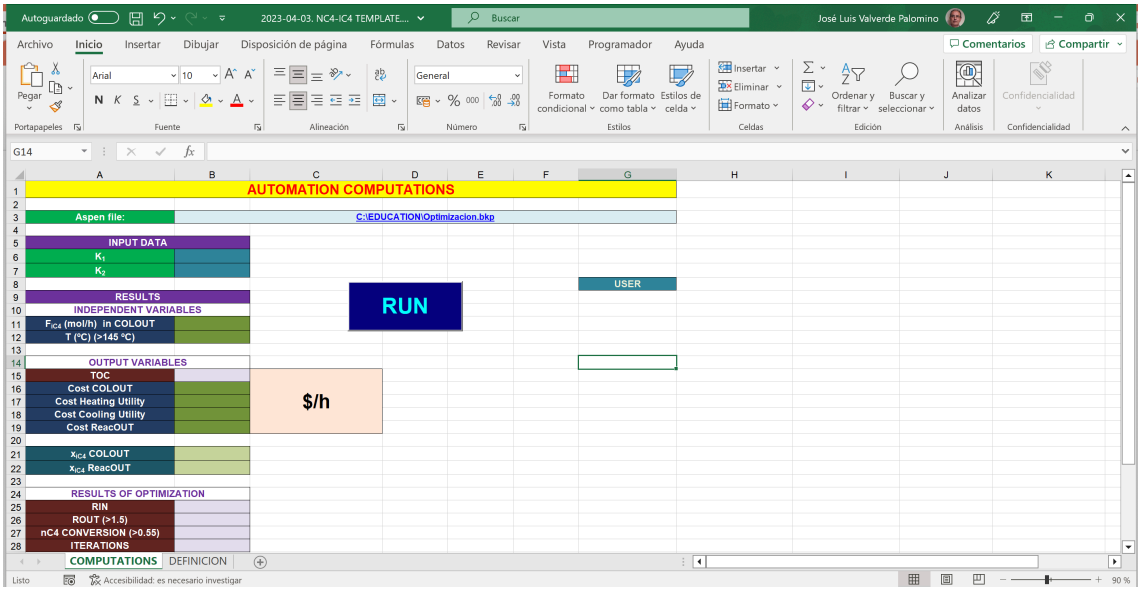


Figure S7. Sheet COMPUTATIONS in the MS EXCEL-VBA template used in Case of Study 3.

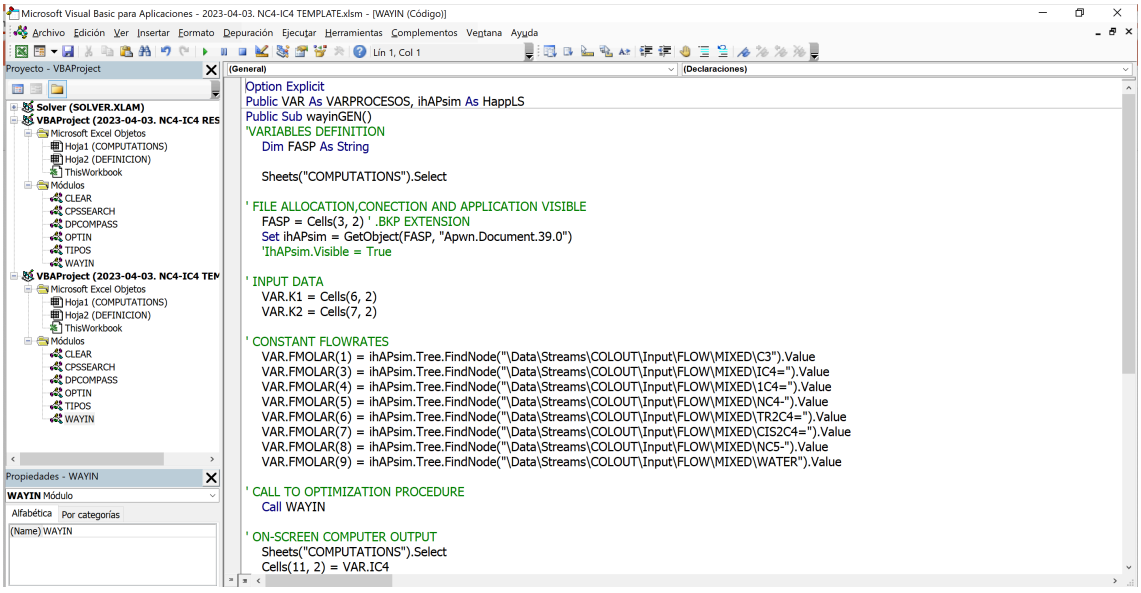


Figure S8. Definition of module WAYIN used in Case of Study 3.

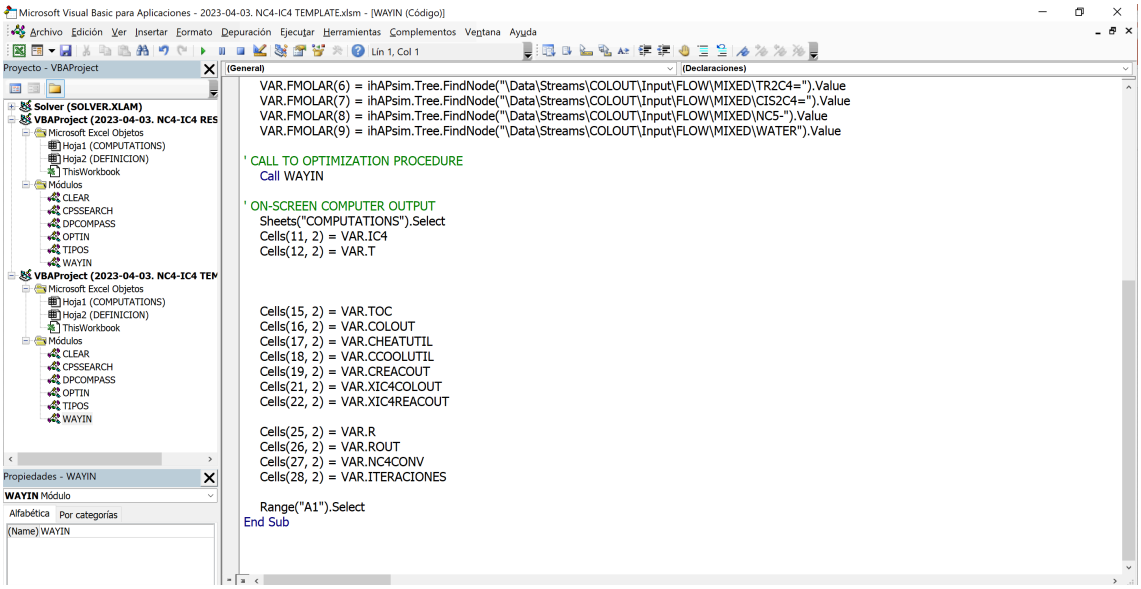


Figure S8. Definition of module WAYIN used in Case of Study 2 (continuation).

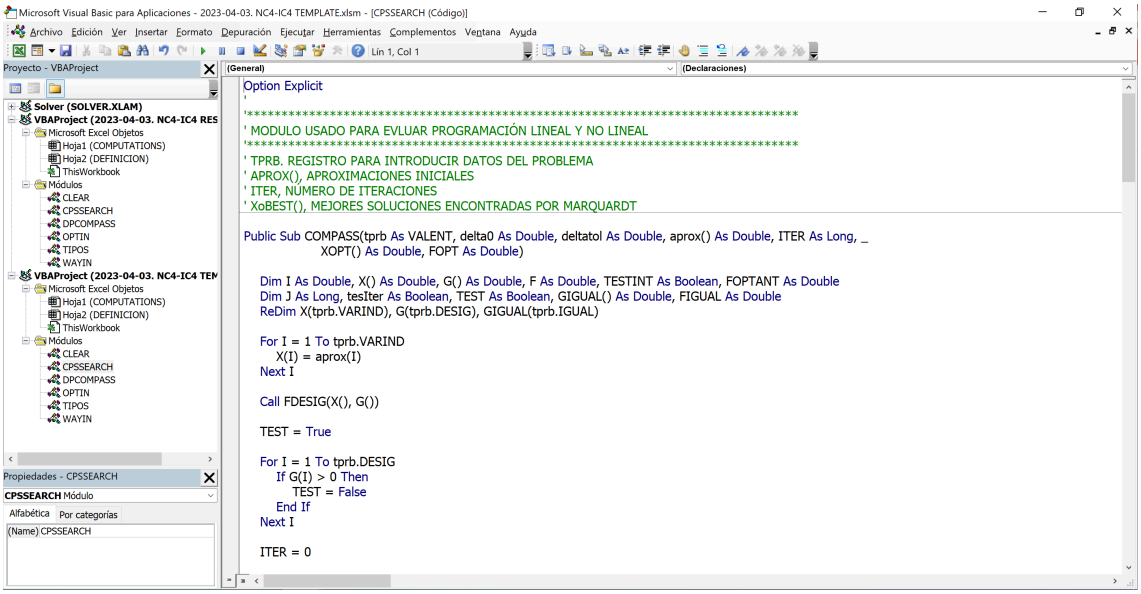


Figure S9. Definition of module OPTIN used in Case of Study 3.

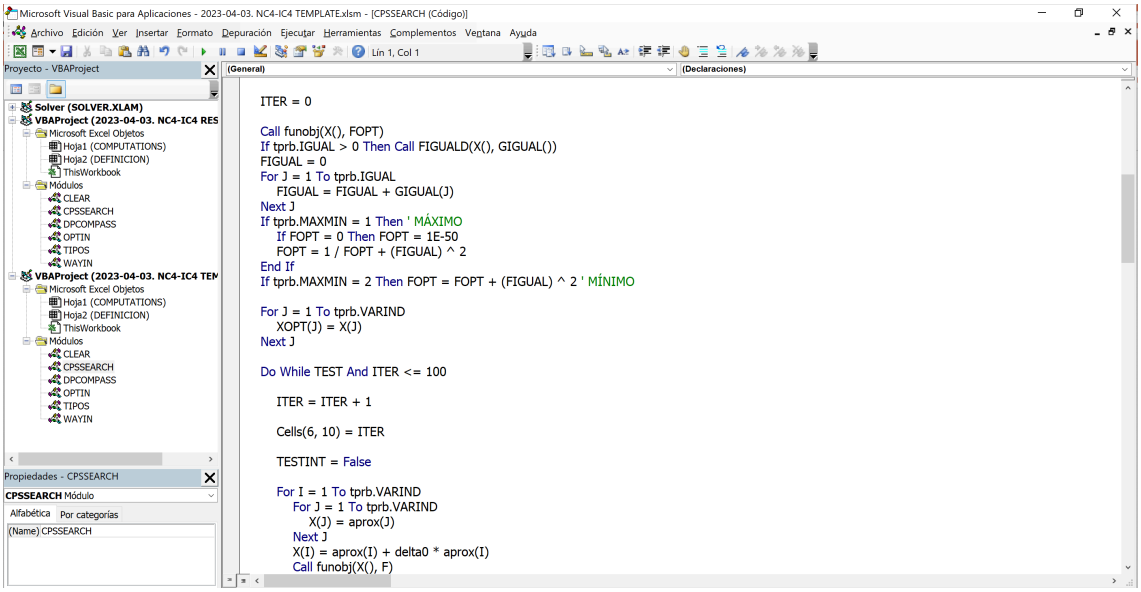


Figure S9. Definition of module OPTIN used in Case of Study 3 (continuation).

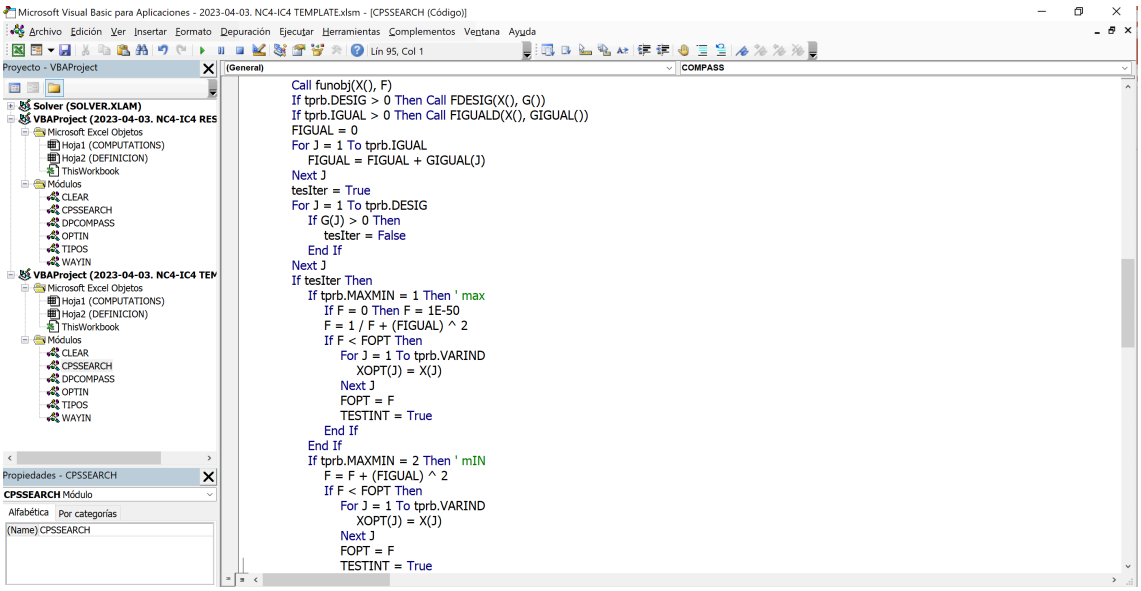


Figure S9. Definition of module OPTIN used in Case of Study 3 (continuation).

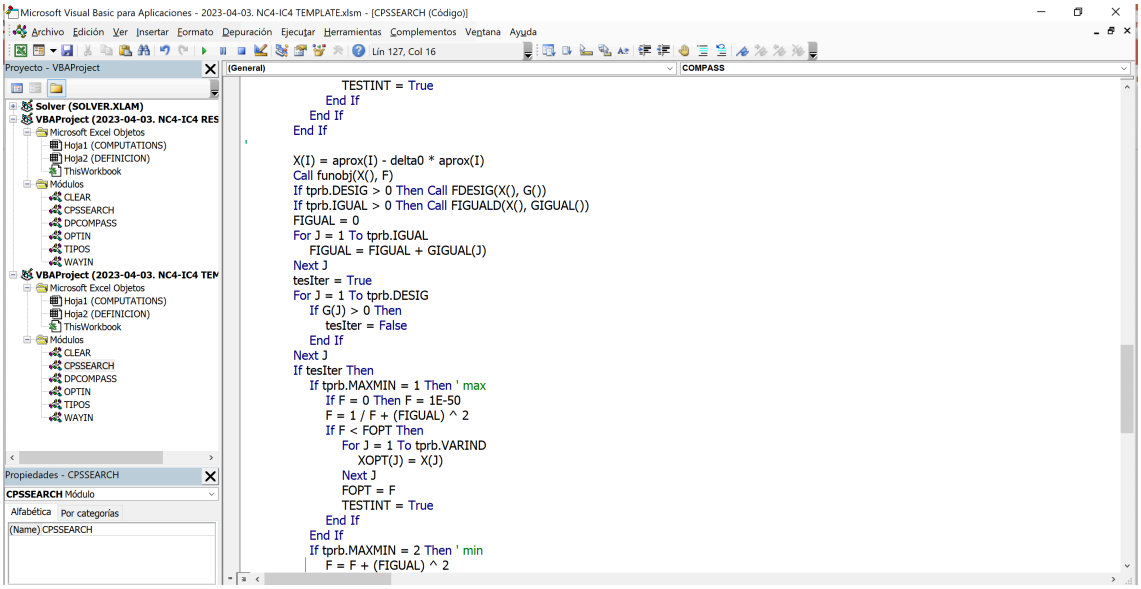


Figure S9. Definition of module OPTIN used in Case of Study 3 (continuation).

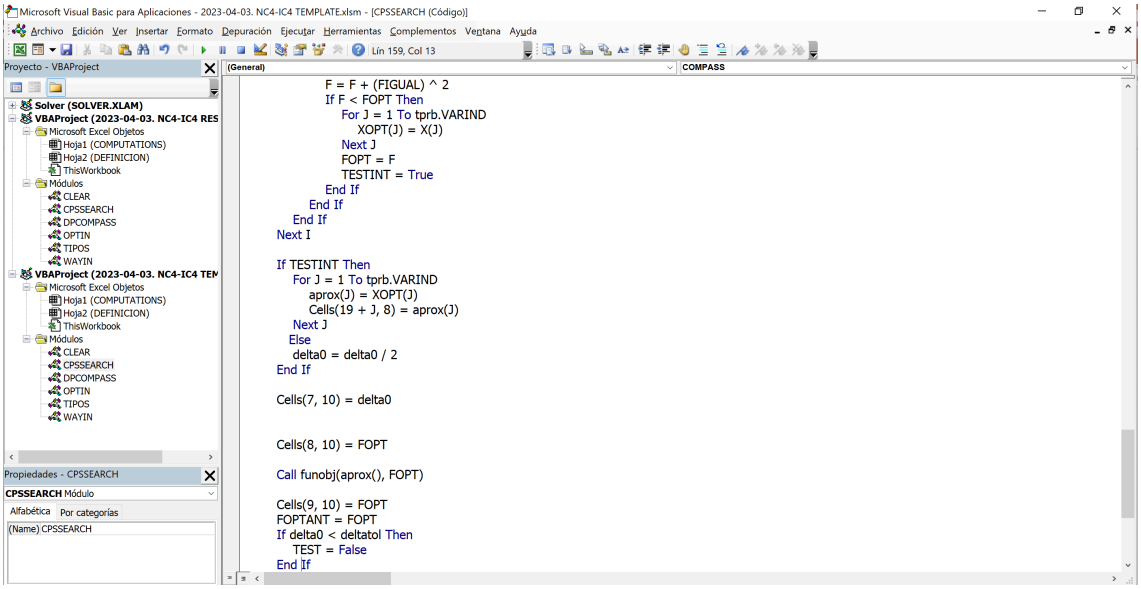


Figure S9. Definition of module OPTIN used in Case of Study 3 (continuation).

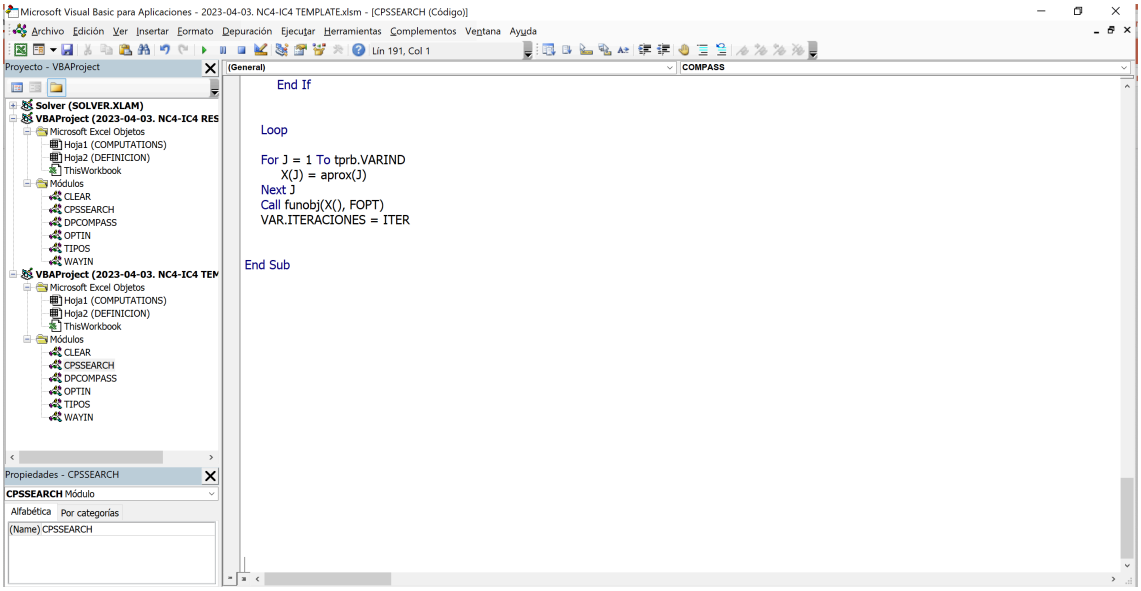


Figure S9. Definition of module OPTIN used in Case of Study 3 (continuation).

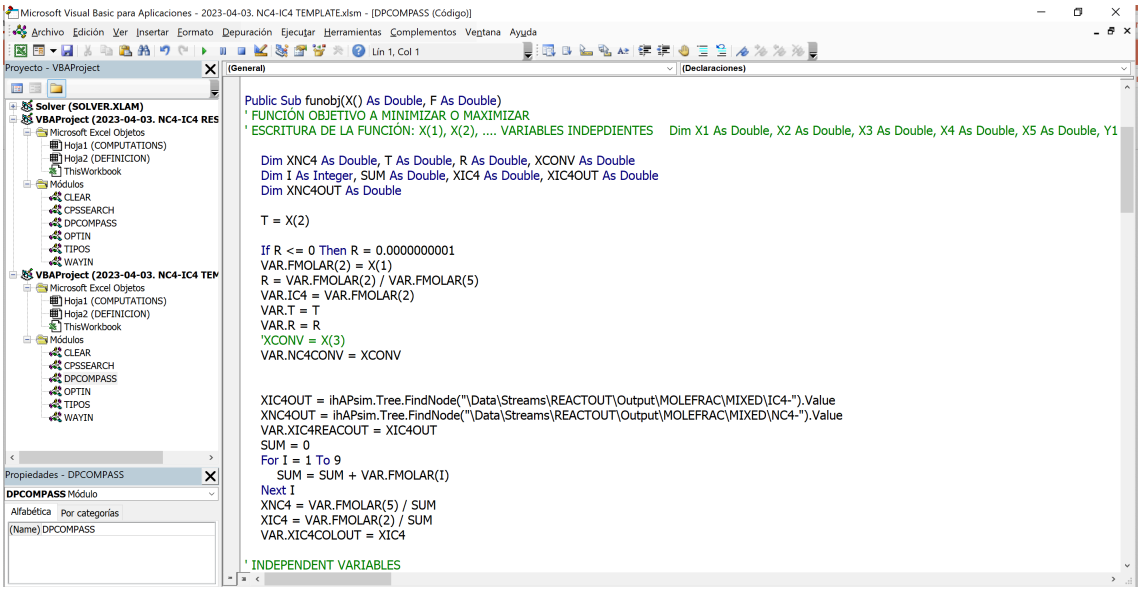
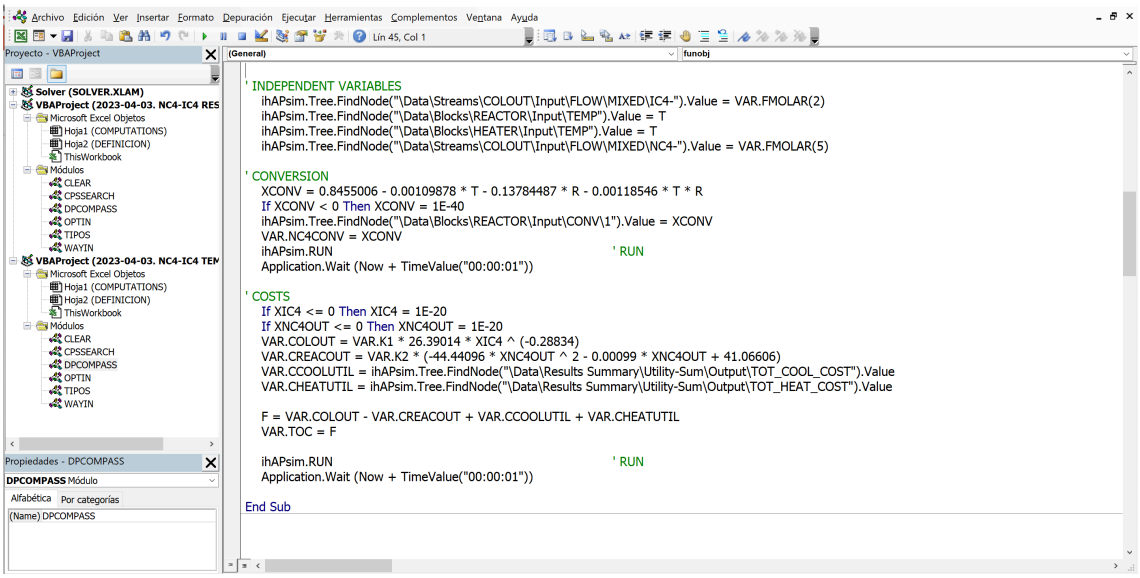
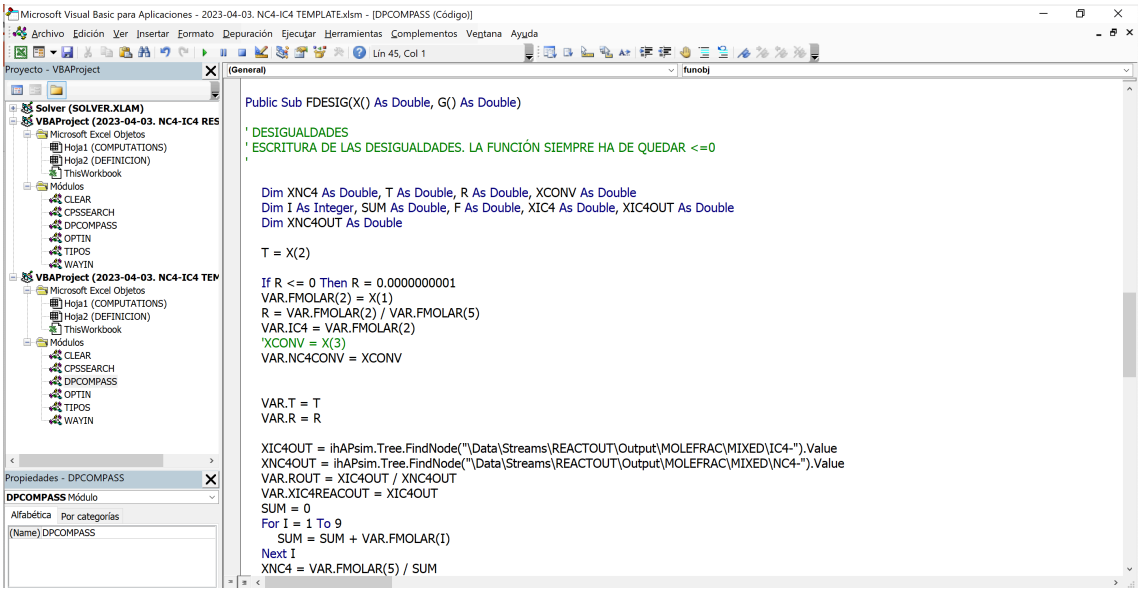


Figure S10. Definition of module DPCOMPASS used in Case of Study 3.



```
' INDEPENDENT VARIABLES
    ihAPsim.Tree.FindNode("\Data\Streams\COLOUT\Input\FLOW\MIXED\IC4-").Value = VAR.FMOLAR(2)
    ihAPsim.Tree.FindNode("\Data\Blocks\REACTOR\Input\TEMP").Value = T
    ihAPsim.Tree.FindNode("\Data\Blocks\HEATER\Input\TEMP").Value = T
    ihAPsim.Tree.FindNode("\Data\Streams\COLOUT\Input\FLOW\MIXED\NC4-").Value = VAR.FMOLAR(5)

' CONVERSION
    XCONV = 0.8455006 - 0.00109878 * T - 0.13784487 * R - 0.00118546 * T * R
    If XCONV < 0 Then XCONV = 1E-40
    ihAPsim.Tree.FindNode("\Data\Blocks\REACTOR\Input\CONV\1").Value = XCONV
    VAR.NC4CONV = XCONV
    ihAPsim.RUN                                          ' RUN
    Application.Wait (Now + TimeValue("00:00:01"))

' COSTS
    If XIC4 <= 0 Then XIC4 = 1E-20
    If XNC4OUT <= 0 Then XNC4OUT = 1E-20
    VAR.COLOUT = VAR.K1 * 26.39014 * XIC4 ^ (-0.28834)
    VAR.CREACOUT = VAR.K2 * (-44.44096 * XNC4OUT ^ 2 - 0.00099 * XNC4OUT + 41.06606)
    VAR.CCOOLUTIL = ihAPsim.Tree.FindNode("\Data\Results Summary\Utility-Sum\Output\TOT_COOL_COST").Value
    VAR.CHEATUTIL = ihAPsim.Tree.FindNode("\Data\Results Summary\Utility-Sum\Output\TOT_HEAT_COST").Value

    F = VAR.COLOUT - VAR.CREACOUT + VAR.CCOOLUTIL + VAR.CHEATUTIL
    VAR.TOC = F

    ihAPsim.RUN                                          ' RUN
    Application.Wait (Now + TimeValue("00:00:01"))

End Sub
```

Figure S10. Definition of module DPCOMPASS used in Case of Study 3 (continuation).



```
Public Sub FDESIG(X() As Double, G() As Double)

' DESIGUALDADES
' ESCRITURA DE LAS DESIGUALDADES. LA FUNCIÓN SIEMPRE HA DE QUEDAR <=0
'

    Dim XNC4 As Double, T As Double, R As Double, XCONV As Double
    Dim I As Integer, SUM As Double, F As Double, XIC4 As Double, XIC4OUT As Double
    Dim XNC4OUT As Double

    T = X(2)

    If R <= 0 Then R = 0.0000000001
    VAR.FMOLAR(2) = X(1)
    R = VAR.FMOLAR(2) / VAR.FMOLAR(5)
    VAR.IC4 = VAR.FMOLAR(2)
    'XCONV = X(3)
    VAR.NC4CONV = XCONV


    VAR.T = T
    VAR.R = R

    XIC4OUT = ihAPsim.Tree.FindNode("\Data\Streams\REACTOUT\Output\MOLEFRAC\MIXED\IC4-").Value
    XNC4OUT = ihAPsim.Tree.FindNode("\Data\Streams\REACTOUT\Output\MOLEFRAC\MIXED\NC4-").Value
    VAR.ROUT = XIC4OUT / XNC4OUT
    VAR.XIC4REACOUT = XIC4OUT
    SUM = 0
    For I = 1 To 9
        SUM = SUM + VAR.FMOLAR(I)
    Next I
    XNC4 = VAR.FMOLAR(5) / SUM
```

Figure S10. Definition of module DPCOMPASS used in Case of Study 3 (continuation).

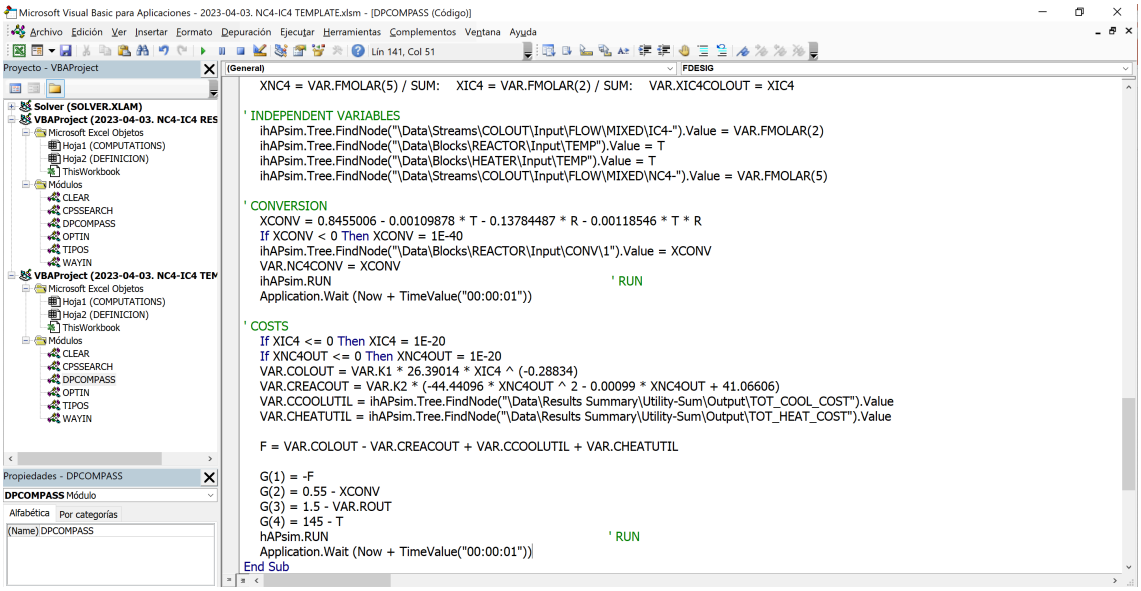


Figure S10. Definition of module DPCOMPASS used in Case of Study 3 (continuation).