

**“A picture is worth a thousand words”**  
(or thousands of chemical reactions)

A new feature in Kintecus 2025 is the ability to generate pictorial plots of the chemical kinetic mechanism with one switch (“-chemnet”). Many examples are shown below after this section. This plotting is accomplished by utilizing the Graphviz graph language[1]. This plotting ability requires the Graphviz system to be located within the “./Kintecus/” directory such as “C:\Kintecus\Graphviz\\*” and the related binaries such as “C:\Kintecus\Graphviz\bin\dot.exe” and “C:\Kintecus\Graphviz\neato.exe” and many other programs. If Graphviz is not present, please download the Windows (or Linux) version and extract the system into the “./Kintecus/” path such as “C:\Kintecus\”

Kintecus can generate such pictures by including a simple switch: “-chemnet”. The actual picture-generating system utilized is the famous graphviz system [1]. Kintecus will generate specialized graphviz test files (that are named “chemnetout.gv”) that graphviz will parse into a chemical network picture. However, most users will want to alter Kintecus ability to output the picture description file to the graphviz system. This is done by including two *optional* test files: a “chemnet.txt” file and/or a “specnet.txt” file. The first optional file, “chemnet.txt,” describes various global values for the picture layer, including network type, network layout, arrow types, reaction types, preprocessors, box color, box type, and much more. The second optional file, “specnet.txt”, applies various filters to the species drawn in the picture, such as “absorbing” some species into the reaction arrow, hiding certain reactants/products, and highlighting sources and sinks for some species. All these features are described in the following two sections. Note that if a user performs a “Mechanism Validation Analysis” on the chemical network via the “-MECHV” switch (described elsewhere in this Kintecus manual) and a “-chemnet” switch is also provided, then Kintecus will generate a picture and *highlight* the four invalid types of illegal loops (if any are present). This graphical highlighting of illegal reaction loops is described below with examples. The picture or vector drawing outputs should be in the same directory as the Kintecus binary (usually in “C:\Kintecus\” and might be named as “C:\Kintecus\chemnetwork.png” or “C:\Kintecus\chemnetwork.svg”).

## The ChemNet Optional File

The ChemNet file, “chemnet.txt”, is optional. This text file contains “key=value” pairs that set various global values for the picture generation. Lines that begin with “#” are treated as comments. The keywords and their default values are shown in the table below.. All keywords are optional.

Table 1. Optional Keywords utilized in the optional Chemnet file "chemnet.txt".

KEYWORD	WHAT DOES IT DO?	POSSIBLE VALUES	DEFAULT VALUE
<b>RENDER</b>	Select the type of Renderer	<b>dot, neato, fdp, circo, sfdp, twopi, nop, nop2, osage.</b> See graphviz documentation.	<b>dot</b>
<b>TYPE</b>	Chemical network display	Species (there is only one option right now)	<b>species</b>
<b>LAYOUT</b>	Distribution of species nodes	Topbottom, leftright, rightright, bottomtop, circular	<b>leftright</b>
<b>OUTSIDE</b>	Set graphic enclosure about species name	Box, circle, oval, diamond, rounded, none	<b>box</b>
<b>ARROW</b>	Display reaction numbers above arrow	1=Ordinal reaction number, 2=Actual line numbers, 0=none	<b>None (0)</b>
<b>REACTION_TYPE</b>	If reaction numbers are displayed, how to display them above the arrow	0=just the reaction number, 1=prefix with character "k<number>", 2=add "k <number>" (note the space). Use this with the ARROW keyword described above in this table.	<b>0</b>
<b>PREPROCESSOR</b>	Select a special network preprocessor ( <i>see below for further information</i> )	pre+postprocessor(s)=0 (none), 1, 2, 3, 4 or 5	<b>0 (none)</b>
<b>FILLCOLOR</b>	Fillcolor for graphic enclosure around species names	black   white   gray   blue   red   purple   green   yellow	<b>white</b>
<b>LINECOLOR</b>	Color for reaction lines	black   white   gray   blue   red   purple   green   yellow	<b>black</b>
<b>SIGN</b>	Select how the species names written on reaction lines are displayed ( <i>see below for more information</i> )	standard   flip   none   R<character_to_use>   P<character_to_use>	<b>standard</b>
<b>ARROW_TYPE</b>	Selects the type of graphic arrow for reactions	vectors (default) , line (none), diamond (diamond ends), circle (circle ends) box, curve, inv, crow, tee (supervector), vee	<b>vectors</b>
<b>OUTPUT</b>	Output the chemical network picture into various picture formats	png (default), jpg, gif, svg (vector drawing), json, ps, pdf, imap, cmapx or fig	<b>png</b>
<b>LINK</b>	Link forward and reverse reactions into a single double arrow	Yes or No	<b>No</b>

The below chemical mechanism of enzyme inhibition will be utilized to describe some basic ChemNet features and all the following sample pictures (please see the “Chemnet\_Enzyme\_Inhibition\_model.xlsm” file):

*Table 2. Enzyme Chemical Mechanism utilized in ChemNet output pictures described below.*

<b>Non-competitive Inhibition of an enzymatic reaction</b>
<b><math>E+S \rightleftharpoons ES</math></b>
<b><math>ES \rightleftharpoons E+S</math></b>
<b><math>E+I \rightleftharpoons EI</math></b>
<b><math>EI \rightleftharpoons E+I</math></b>
<b><math>ES+I \rightleftharpoons EIS</math></b>
<b><math>EIS \rightleftharpoons ES+I</math></b>
<b><math>EI+S \rightleftharpoons EIS</math></b>
<b><math>EIS \rightleftharpoons EI+S</math></b>
<b><math>EI+P \rightleftharpoons EIS</math></b>
<b><math>EIS \rightleftharpoons EI+P</math></b>
<b><math>ES \rightleftharpoons E+P</math></b>

and we will use this ChemNet description file as a start:

```

#
# Parameters for Kintecus Visual Graph of Kinetic System
# (invoked with the "-chemnet:chemnet.txt" or "-chemnet" switch)
#
# All keywords are OPTIONAL and Keywords can be in any order
#
# RENDER
# Select the type of Renderer=dot[default], neato, fdp, circo, sfdp, twopi, nop, nop2, osage
render=dot
#
# TYPE
# type=species
type=species
#
# LAYOUT
# layout=topbottom, leftright [default], rightleft, bottomtop, circular
layout=leftright
#
# Outside enclosure
# Outside=box [default], circle, oval, diamon, rounded, none
outside=rounded
#
# ARROW
# 1=reaction numbers, 2=actual line numbers [default]
ARROW=1
#
# REACTION_TYPE
# 0=just the reaction number [default], 1=prefix with character "k<number>", 2=add "k <number>"
# arrow_type=Reaction # | k | k_SPACE
Reaction_Type=k
#
# Preprocessing and Postprocessing
# pre+postprocessor(s)=0 (none), 1, 2, 3, 4 or 5
preprocessor=0
#
# FILLCOLOR
# fillcolor=black, white [default], gray, blue, red, purple, gree, yellow
fillcolor=yellow
#
# LINECOLOR
# linecolor=black[black], white, gray, blue, red, purple, green, yellow
linecolor=black
#
# SIGN
# sign= standard | flip | none | R<character_to_use> | P<character_to_use>
# standard will place a minus sign in front of reactant species names only
# and a plus, "+" in front of the reactions product's species names t
# flip : flips the signage on the reactants and products species names
# R<character> will use the single <character> in front of the reactions reactant species names
# (the product species names in the arrows with have space or nothing in front of them)
# P<character> will use the single <character> in front of the reactions prodcut species names
# (the reactant species names in the arrows with have space or nothing in front of them)
sign=flip
#
#
# Arrow_type=vectors (default) , line (none), diamond (diamond ends), circle (circle ends)
# box, curve, inv, crow, tee, vee
Arrow_type=vee
#
# Output type
# Select either png (default), jpg, gif, svg, json, ps, pdf, imap, cmappx or fig
#
Output=jpg
#
# Combine reversible reactions into a single DOUBLE error
LINK=YES
#

```

And this is the optional Specnet description file:

# Species	Arrow Placement	Display Filter	Source Color	Sink Color
# Name	(0,1,2,3)	(0,1,2,3,4,5,6)		
I	3		0 black	black
S	3		0 black	black
<b>END</b>				

Note that the species "I" and "S" have the value "3" set in their "Arrow Placement" column in the SpecNet input file ("specnet.txt" and described in further detail below), indicating to Kintecus to place those two species into the reaction arrow and do not create a species node for them. The created picture is shown below. Although the "Render" keyword has a few options, the most important to know are the "dot", "neato", "sfdp", and "circo" keywords as shown below (no other changes were made to ChemNet nor Specnet files):

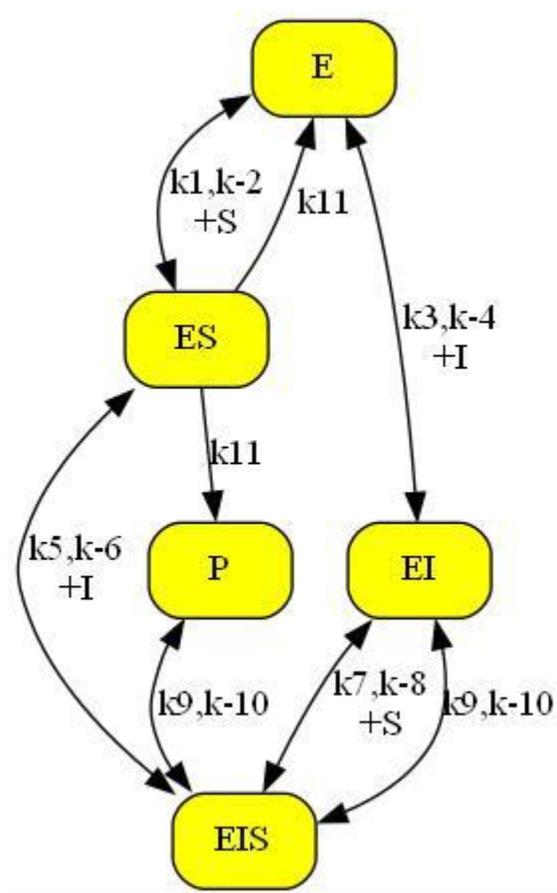


Figure 1. A Chemnet visualization of the reactions listed in Table 2 above, "Enzyme Chemical Mechanism" with Render="dot"

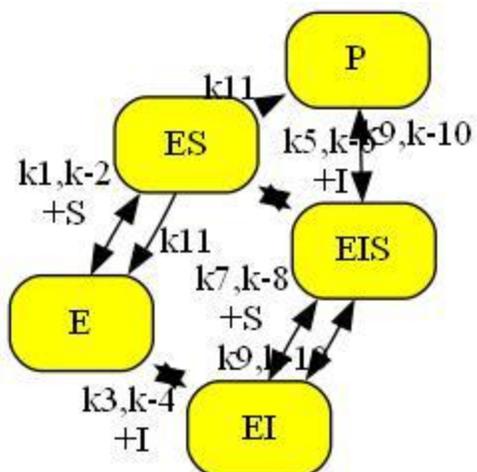


Figure 2. A Chemnet visualization of the reactions listed in Table 2 above, "Enzyme Chemical Mechanism" with Render="neato"

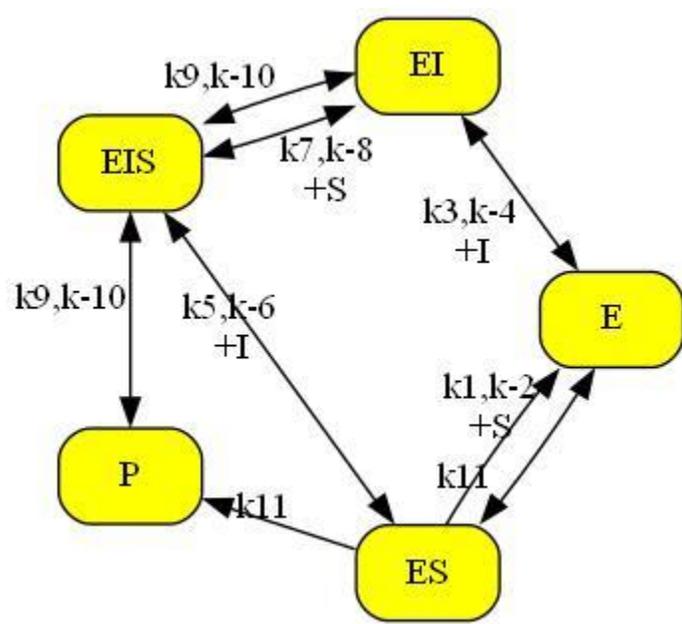


Figure 3. A Chemnet visualization of the reactions listed in Table 2 above, "Enzyme Chemical Mechanism" with Render="circo"

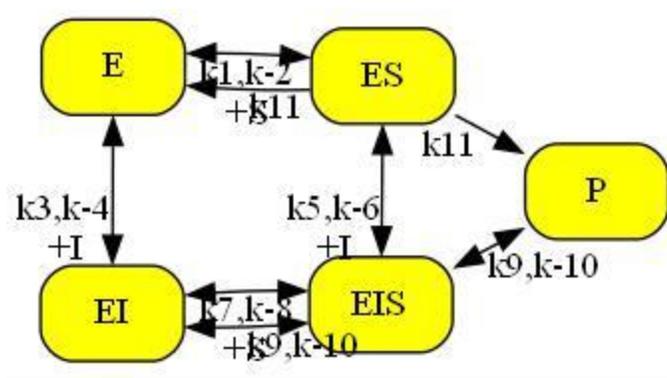


Figure 4. A Chemnet visualization of the reactions listed in Table 2 above, “Enzyme Chemical Mechanism” with Render=sfdp

Although the “layout” keyword supports various display features, the most useful are top-to-bottom (topbottom) and Left-to-right (leftright):

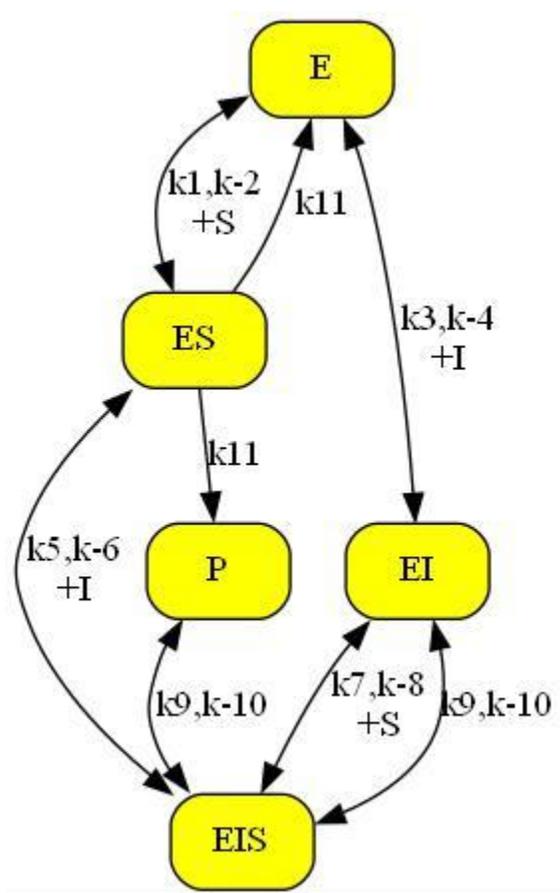


Figure 5. A Chemnet visualization of the reactions listed in Table 2 above, “Enzyme Chemical Mechanism” with Layout=topbottom

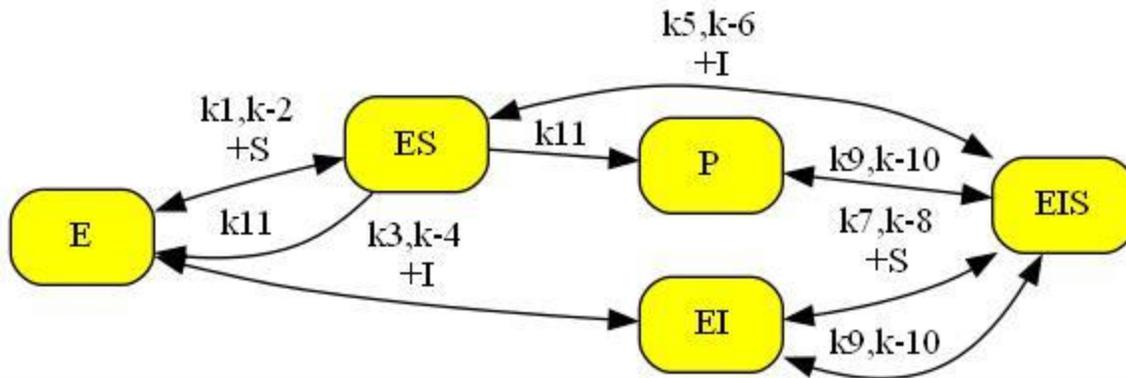


Figure 6. A Chemnet visualization of the reactions listed in Table 2 above, "Enzyme Chemical Mechanism" with *Layout=leftright*

Changing the "sign=standard" and "link=no" in the ChemNet file and rerunning using the same left-to-right layout as shown above, we now get:

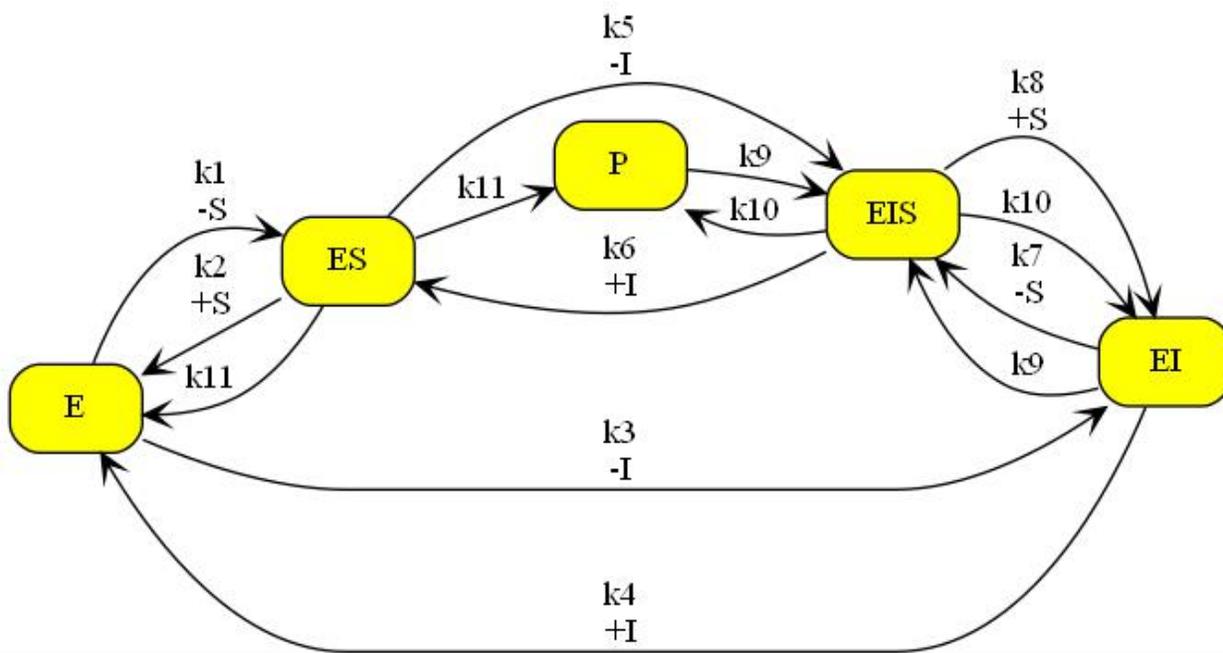


Figure 7. A Chemnet visualization of the reactions listed in Table 2 above, "Enzyme Chemical Mechanism" with *Sign=standard*, and no linking (*LINK=no*) of forward/reverse reactions. Note the sign of "S" and "I" in the reaction arrows and the presence of more reaction arrows.

Note the double ended reaction arrows have been replaced with individual single ended reaction arrows. We can also hide species in the plot:

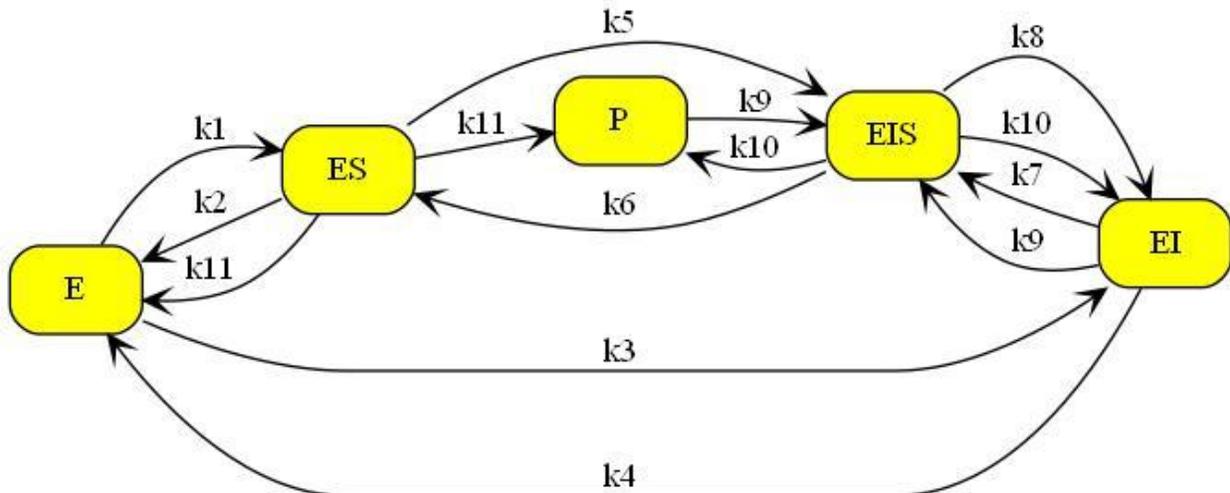


Figure 8. A Chemnet visualization of the reactions listed in Table 2 above, “Enzyme Chemical Mechanism” using the previous plot, the species “I” and “S” are not displayed anywhere by using the Display Filter for species “I” and “S” to a value of “3”. This is described in more detail in the SpecNet section below.

The figure above shows the complete absence of the species “I” and “S”. This is accomplished by setting their display filter to “3” for species “I” and “S” in the Specnet spreadsheet (further described below):

# Species	Arrow Placement	Display Filter	Source Color	Sink Color
# Name	(0,1,2,3)	(0,1,2,3,4,5,6)		
I	0	3	black	black
S	0	3	black	black
<b>END</b>				

As hinted above, the SIGN keyword changes how the “+” or “-” is interpreted when displaying a species above the arrow. In the literature, a prefixed “+” before a species name sometimes translates into “add this reactant.” In other literature areas the plus, “+”, is interpreted as a product that is formed (such as in some atmospheric journals). Kintecus allows the switching of this interpretation by assigning the +/- sign to “standard” or “flip”. One can also use other characters to represent a reactant prefixed with a minus, “-”, and the product as a *<space>* by assigning “SIGN=R-” or a product prefixed with a minus, “-”, with “SIGN=P-” or an ampersand, “SIGN=P&”.

The ARROW key accepts three values 0-2. Zero, “0” does not place any numbers above the reaction arrows. A value of one, “1”, will place the ordinal line numbers (if you deleted all the comments in the MODEL spreadsheet and counted from the top) above the reaction arrows. Setting the ARROW field to two, “2”, which will place the actual line numbers in your MODEL worksheet for the reaction’s arrows above the reaction arrows. The value two, “2” is the default for the ARROW keyword.

The Reaction\_Type keyword accepts three values, 0-2 and will prefix the reaction numbers with nothing, “k<number>” or “k<space><number>” respectively.

As mentioned above, the "LINK" keyword will combine the backward and forward arrows for reactions into a single double arrow. This linking of forward and backward reaction arrows into a single double-sided arrow can reduce the clutter in larger chemical network plots.

The output of the ChemNet network is a png file as the default. There are many other output picture formats such as jpg, gif, svg, ps, pdf or fig. Please see the graphviz manual for more explanation of the outputs.

It is **very important** to note that if one uses the Kintecus-Excel workbooks, the workbook will automatically **delete** any **previous** "chemnetwork.png" or "chemnetwork.jpg" and "chemnet.txt" or "specnet.txt" files once you click "RUN" on the CONTROL worksheet! Be sure to move/copy those files to a different area or rename them to a different filename!

The preprocessor keyword supports five different values, 0-4. This keyword utilizes several graphviz pre- and postprocessing options to condense networks. Selecting zero performs no network pre- or post-analysis. The preprocessors produce almost no change for simple models like this enzyme inhibition model. For example, preprocessor 3 (setting "preprocessor=3"), "flattens" graphs by looking at one path and deleting redundant paths, so our initial enzyme model becomes:

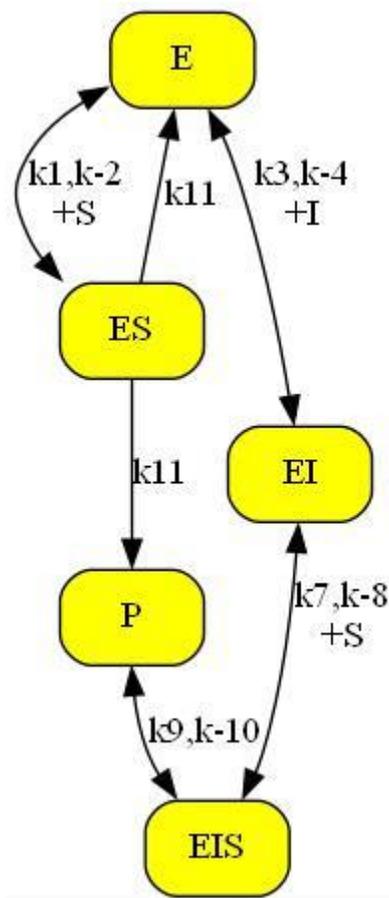


Figure 9. A Chemnet visualization of same Table 3 above, "Enzyme Chemical Mechanism" with "preprocessor=3"

Again, keep in mind that the final picture output should be in the same directory as the Kintecus binary (usually in "C:\Kintecus\" and might be named as "C:\Kintecus\chemnetwork.png" or "C:\Kintecus\chemnetwork.svg").

**IMPORTANT!** Note that if one uses the Kintecus-Excel worksheets, any previous chemnetwork.png or chemnetwork.jpg files will automatically be DELETED once one clicks the "RUN" button on the CONTROL worksheet! One should move/copy those files to a different area or rename them to a different filename!

## The Specnet Optional File

The Specnet, "specnet.txt", file is optional. The Specnet file will apply filters and changes to the species drawn in the picture, such as "absorbing" some species into the reaction arrow, hiding certain reactants/products, and highlighting sources and sinks for the user's selected species. The Specnet file has five fields: "Species name", "Arrow Placement", "Display Filter", "Source Color" and "Sink Color":

# Species	Arrow Placement	Display Filter	Source Color	Sink Color
# Name	(0,1,2,3)	(0,1,2,3,4,5,6)	(black, blue, red, green, gray, purple)	(black, blue, red, green, gray, purple)
# This is a sample specnet.txt input file				
#				
# <b>Arrow Placement field values ==</b> 0 Do not show as part of reaction arrow, 1 show in arrow if reactant, 2 show in arrow if product, 3 show in arrow if either reactant/product				
#				
# <b>Display_Filter</b> can take several values == 0=SHOW; 1=If reactant do not show anywhere; 2=If product do not show anywhere; 3=DO NOT SHOW AT ALL				
# 4=ONLY_SHOW_REACTANT,5=ONLY_SHOW_PRODUCT,6=ONLY_REACTANT_PRODUCT				
#				

Adding a species to the "Species Name" column is optional. If a species is listed here, it **MUST** be defined in the "Species Description Spreadsheet" file. Please remember that the species listed in the "Species Description Spreadsheet" must match **exactly** the same species name in the SpecNet file, as the names are **CaSe SeNsItIvE**.

The Source and Sink color fields should be obvious and they can contain the values, "black, blue, red, green, gray, purple, yellow". Reaction arrows that point to a species (a source) will be colored as stated in the source color field for that species name. Reaction arrows that point away from a species (a sink) will be colored as stated in the sink color field for that species' name. If more than one species has a source or sink color, then the species listed first will have that color and override other species down on the list.

The "Arrow\_Placement" forces whether a species is "absorbed" into the reaction arrow. This field contains four possible values: 0, 1, 2, 3:

- 1) "0" do not place the species into a reaction arrow.
- 2) "1" place the species into a reaction arrow if it appears as a reactant in any reaction
- 3) "2" place the species into a reaction arrow if it appears as a product in any reaction
- 4) "3" place the species into a reaction arrow if it shows up as either a reactant or product in a reaction

When a species is displayed above a reaction arrow, the sign (such as minus, "-", prefixed in front of a reactant for a reaction) of the species is dictated by the "SIGN" option described in the ChemNet file. Placing certain "background" or "passenger" chemical species (such as H<sup>+</sup>, H<sub>2</sub>O, N<sub>2</sub>, M, Cl<sup>-</sup>, Br<sup>-</sup>, etc) can *significantly* reduce the "clutter" in a chemical network graph.

The "Display Filter" field states whether to show a species or whether to not to show *other* species or not.

- 1) "0" show the species
- 2) "1" if the species is a reactant, then **do not** show it anywhere in the picture.
- 3) "2" if the species is a product, then **do not** show it anywhere.
- 4) "3" if the species is a reactant or product, then do not show it anywhere
- 5) "4" show **ONLY** this species in reactants(!!)
- 6) "5" show **ONLY** this species in products(!!)
- 7) "6" show **ONLY** this species in products or reactants(!!)

Setting this field to values of four, "4" or above, can drastically change the picture, as it turns off the display of any species that are *not directly related to the said species*. Values of "3" might be used for species that appear throughout a reaction mechanism. They are not necessary in the visualization of a chemical scheme such as "M" (Loschmidt's number), "H<sup>+</sup>", "H<sub>2</sub>O", "CO<sub>2</sub>", etc., and can be ignored in larger mechanisms. If one were only interested in viewing all the direct sources or sinks for CO<sub>2</sub> and H<sub>2</sub>O in a large chemical mechanism, one would set the "Display\_Filter" for the CO<sub>2</sub> and H<sub>2</sub>O species to "6." This will hide ALL species that are not direct sources or sinks for CO<sub>2</sub> and H<sub>2</sub>O. Are you confused? Look at the examples below to clarify this further.

A sample Specnet file is shown below. This Specnet file is utilized to plot a chemical network picture of "Photochemical Chlorate-Iodide Clock Reaction", Romulo O. Pires and Roberto B. Faria, *Inorg. Chem.* 2022. The species I<sub>2</sub> is highlighted with a green source arrow and red sink arrows as shown in the figure below. The passenger ions, Chloride (Cl<sup>-</sup>), iodide (I<sup>-</sup>) and I<sub>3</sub><sup>-</sup> are not shown in the picture. This is because those two passenger ions have a "3" in the "Display\_Filter" causing them not to be shown. Hiding such passenger ions can significantly reduce the clutter in large chemical network plots. To further reduce the chemical network clutter, the species, H<sup>+</sup>, H<sub>2</sub>O and HIO<sub>2</sub> are placed into the reaction arrows by placing a "3" in the "Arrow\_Placement" field for the listed species names. Also, the signs of the reactants are negative if they are a product in a reaction and appear in the reaction arrow. This is due to the sign keyword in the Chemnet file is set to the default of "standard". This sign placement is the opposite of the previous enzyme inhibition model samples. The reaction numbers are actually the line numbers the reactions appear on in the MODEL worksheet.

# Species	Arrow Placement	Display Filter	Source Color	Sink Color
# Name	(0,1,2,3)	(0,1,2,3,4,5,6)	(black, blue, red, green, gray, purple)	(black, blue, red, green, gray, purple)
# This is a sample specnet.txt input file # # <b>Arrow Placement field values ==</b> 0 Do not show as part of reaction arrow, 1 show in arrow if reactant, # 2 show in arrow if product, 3 show in arrow if either reactant/product # # <b>Display_Filter</b> can take several values == 0=SHOW; 1=If reactant do not show anywhere; 2=If product do not show anywhere; # 3=DO NOT SHOW AT ALL # 4=ONLY_SHOW_REACTANT,5=ONLY_SHOW_PRODUCT,6=ONLY_REACTANT_PRODUCT #				
I2		0	0 green	red
Cl-		0	3 black	black
H+		3	0 black	black
H2O		3	0 black	black
I-		0	3 black	black
I3-		0	3 black	black
HIO2		3	0 black	black
END				

Figure 10. Specnet file for the picture generation of "Photochemical Chlorate-Iodide Clock Reaction", Romulo O. Pires and Roberto B. Faria, *Inorg. Chem.* 2022

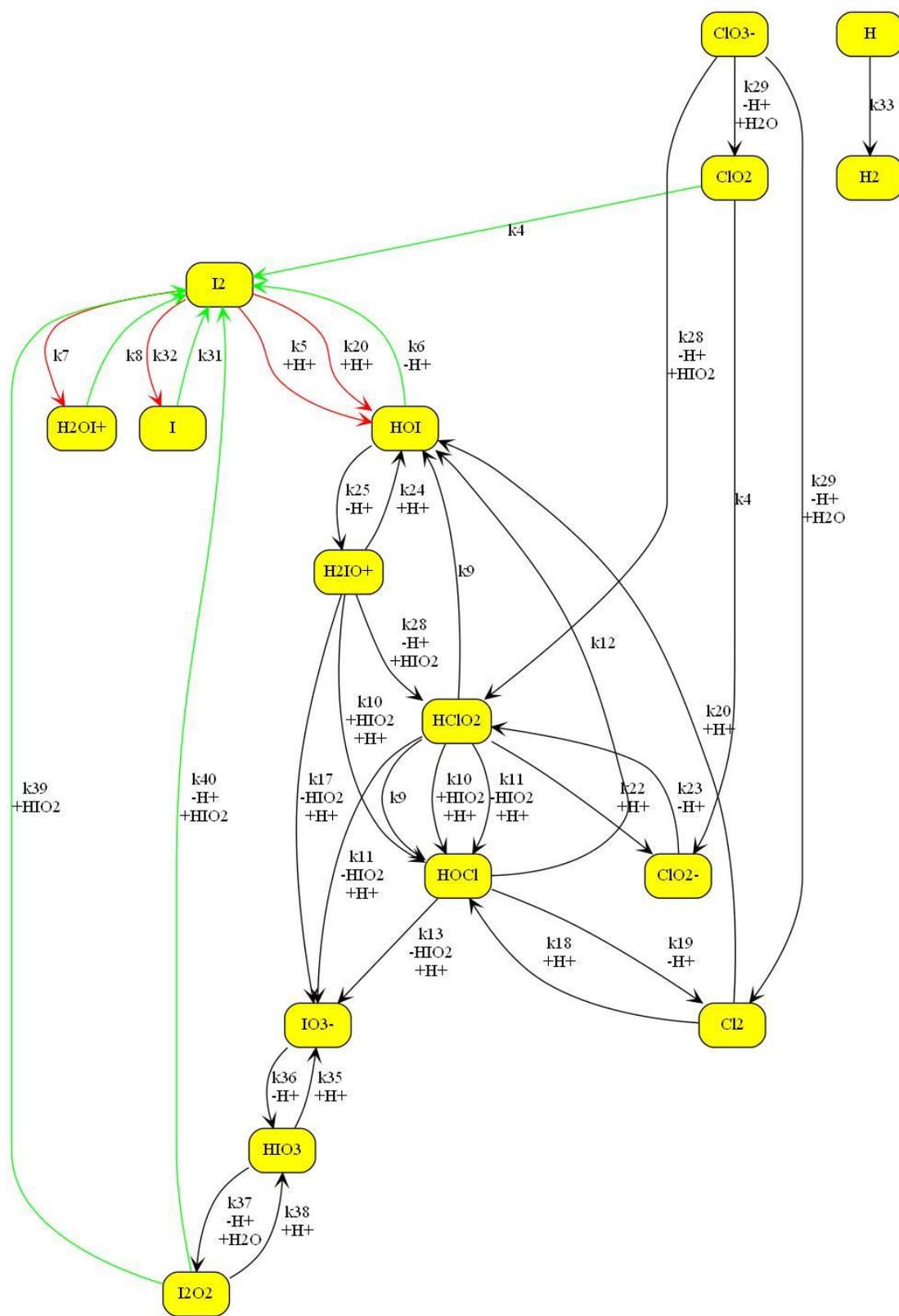


Figure 11. ChemNet picture representation of the "Photochemical Chlorate-Iodide Clock Reaction", Romulo O. Pires and Roberto B. Faria, *Inorg. Chem.* 2022

```

#
# Parameters for Kintecus Visual Graph of Kinetic System
# (invoked with the "-chemnet:chemnet.txt" or "-chemnet:D" switch)
#
# All keywords are OPTIONAL and Keywords can be in any order
#
# RENDER
# Select the type of Renderer=dot, neato, fdp, circo, sfdp, twopi, nop, nop2, osage
render=dot
#
# TYPE
# type=species
type=species
#
# LAYOUT
# layout=topbottom | leftright | rightleft | bottomtop | circular
layout=topbottom
#
# Outside enclosure
# Outside=box|circle|oval|diamond|rounded | none
outside=rounded
#
# ARROW
# 1=reaction numbers, 2=actual line numbers
ARROW=2
#
# REACTION_TYPE
# 0=just the reaction number, 1=prefix with character "k<numbers>", 2=add "k <number>"
# arrow_type=Reaction #|K|K_SPACE
Reaction_Type=K
#
# Preprocessing and Postprocessing
# pre+postprocessor(s)=0 (none), 1, 2, 3, 4 or 5
preprocessor=0
#
# FILLCOLOR
# fillcolor=black|white|gray|blue|red|purple|green|yellow
fillcolor=yellow
#
# LINECOLOR
# linecolor=black|white|gray|blue|red|purple|green|yellow
linecolor=black
#
# SIGN
# sign= standard | flip |none | R<character_to_use> | P<character_to_use>
# standard will place a minus sign in front of reactant species names only
# and a plus, "+" in front of the reactions product's species names t
# flip : flips the signage on the reactants and products species names
# R<character> will use the single <character> in front of the reactions reactant species names
# (the product species names in the arrows with have space or nothing in front of them)
# P<character> will use the single <character> in front of the reactions product species names
# (the reactant species names in the arrows with have space or nothing in front of them)
sign=standard
#
#
# Arrow_type=vectors (default) , line (none), diamond (diamond ends), circle (circle ends)
# box, curve, inv, crow, tee, vee
Arrow_type=vee
#
# Output type
# Select either png (default), jpg, gif, svg, json, ps, pdf, imap, cmapx or fig
#
Output=jpg
#
#
# Combine reversible reactions into a single DOUBLE arrow
LINK=NO
#

```

Figure 12. ChemNet file for the "Photochemical Chlorate-Iodide Clock Reaction", Romulo O. Pires and Roberto B. Faria, *Inorg. Chem.* 2022



# Species	Arrow Placement	Display Filter	Source Color	Sink Color
# Name	(0,1,2,3)	(0,1,2,3,4,5,6)		
HClO <sub>2</sub>	0	6	green	red
H <sup>+</sup>	0	6	green	red
END				

Figure 15. SpecNet file for the **above** plot. Note the values of “6” in the “Display Filter” column. This forces the entire plot to center only around the “HClO<sub>2</sub>” and “H<sup>+</sup>” species sinks and sources.

Note that any source or sink hours from H<sup>+</sup> to HClO<sub>2</sub> are green and red because HClO<sub>2</sub> has a higher priority in color assignment as that species is listed before H<sup>+</sup>.

Let’s look at the H<sub>2</sub>-O<sub>2</sub> combustion model (“ChemNet\_Combustion\_workbook\_OH.xlsm”) and view the paths to H<sub>2</sub>O. We will use this ChemNet file:

```

#
# Parameters for Kintecus Visual Graph of Kinetic System
# (invoked with the "-chemnet:chemnet.txt" or "-chemnet:D" switch)
#
# All keywords are OPTIONAL and Keywords can be in any order
#
# RENDER
# Select the type of Renderer=dot, neato, fdp, circo, sfdp, twopi, nop, nop2, osage
render=dot
#
# TYPE
# type=species
type=species
#
# LAYOUT
# layout=topbottom | lefright | rightleft | bottomtop | circular
layout=lefright
#
# Outside enclosure
# Outside=box|circle|oval|diamond|rounded | none
outside=rounded
#
# ARROW
# 1=reaction numbers, 2=actual line numbers
ARROW=2
#
# REACTION_TYPE
# 0=just the reaction number, 1=prefix with character "k<number>", 2=add "k <number>"
# arrow_type=Reaction #|K|K_SPACE
Reaction_Type=K
#
# Preprocessing and Postprocessing
# pre+postprocessor(s)=0 (none), 1, 2, 3, 4 or 5
preprocessor=0
#
# FILLCOLOR
# fillcolor=black|white|gray|blue|red|purple|green|yellow
fillcolor=yellow
#
# LINECOLOR
# linecolor=black|white|gray|blue|red|purple|green|yellow
linecolor=black
#
# SIGN
# sign= standard | flip |none | R<character_to_use> | P<character_to_use>
# standard will place a minus sign in front of reactant species names only
# and a plus, "+" in front of the reactions product's species names t
# flip : flips the signage on the reactants and products species names
# R<character> will use the single <character> in front of the reactions reactant species names
# (the product species names in the arrows with have space or nothing in front of them)
# P<character> will use the single <character> in front of the reactions prodcut species names
# (the reactant species names in the arrows with have space or nothing in front of them)
sign=standard
#
#
# Arrow_type=vectors (default) , line (none), diamond (diamond ends), circle (circle ends)
# box, curve, inv, crow, tee, vee
Arrow_type=vee
#
# Output type
# Select either png (default), jpg, gif, svg, json, ps, pdf, imap, cmapx or fig
#
Output=jpg
#
#
# Combine reversible reactions into a single DOUBLE error
LINK=YES
#

```

Figure 16.

And this Specnet file:

# Species # Name	Arrow_Placement (0,1,2,3)	Display Filter (0,1,2,3,4,5,6)	Source Color	Sink Color
M	3	0	black	black
O2	3	0	black	black
H2O	0	0	green	red
<b>END</b>				

Which produces this picture:

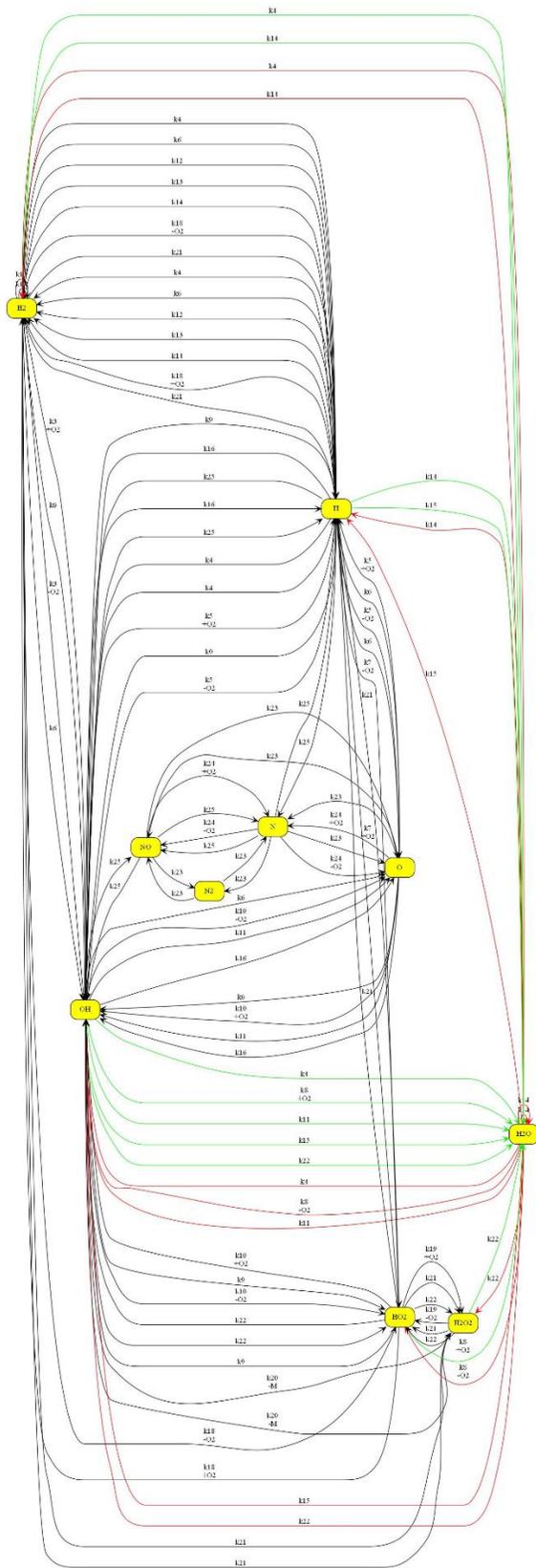


Figure 17.

The plot above is complicated, quite “busy,” and “smooshed.” If we select the “circo” renderer (setting “render=circo” in the ChemNet file) and combining the forward and reverse reactions (set LINK=“yes” in the ChemNet file) and hide O<sub>2</sub> and M (setting the Display\_Filter for O<sub>2</sub> and M to “3” in Specnet file) we get this picture of the same chemical mechanism:

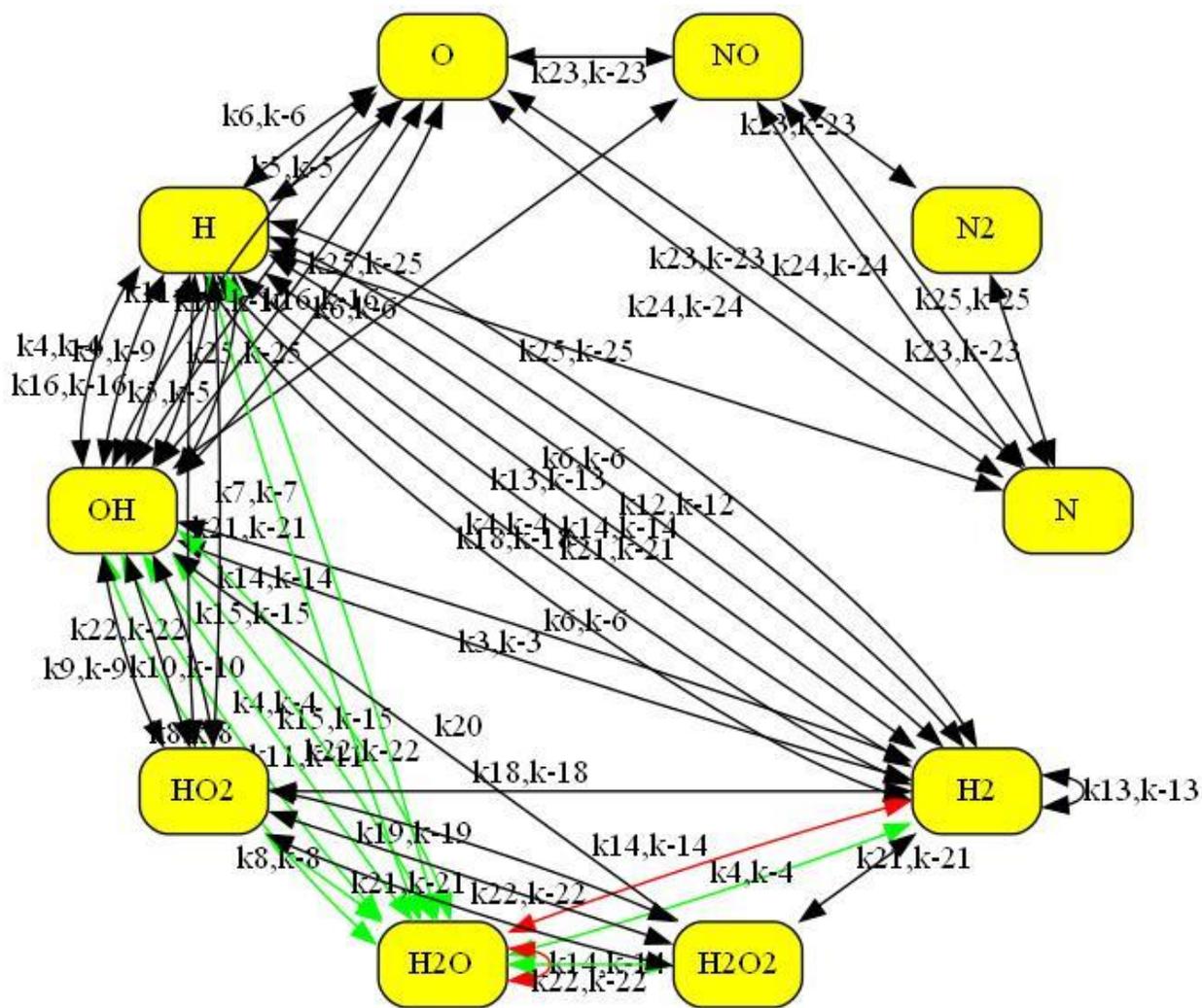


Figure 18. Render="circo" with LINK=YES of the H<sub>2</sub>-O<sub>2</sub> combustion model.

The picture is still little complicated. We could remove the reaction labels on the reaction lines to clear it up. We can also just examine paths to H<sub>2</sub>O by setting the Display\_Filter for H<sub>2</sub>O to “6” yielding this Specnet file:

# Species	Arrow_Placement	Display Filter	Source Color	Sink Color
# Name	(0,1,2,3)	(0,1,2,3,4,5,6)		
M	3	0	black	black
O2	3	0	black	black
H2O	0	6	green	red
END				

This yields a much more compact picture:

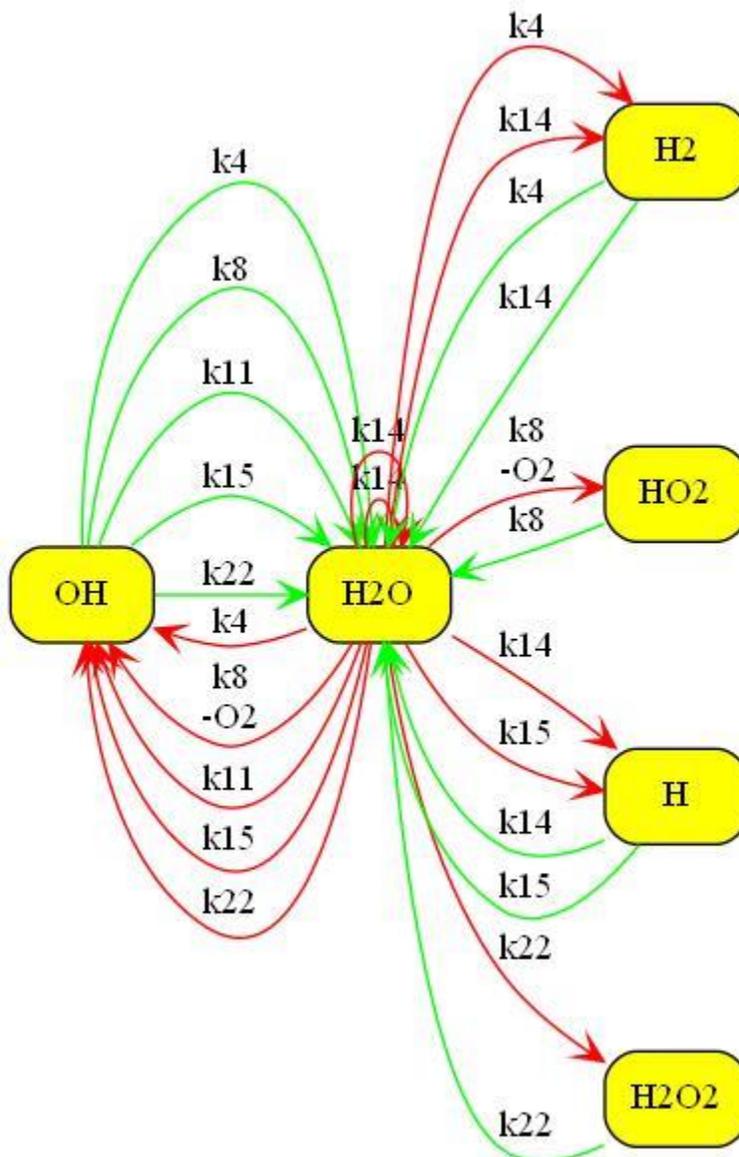


Figure 19. Display\_Filter now set to "6" for H<sub>2</sub>O.

The above plot is much easier to view.

## More Sample Chemnet Plots

The following Chemical Network Description file (ChemNet) settings for the following enzyme inhibition samples are shown in the figure below. Again, all ChemNet keywords are optional and can be in any order. Lines that start with “#” are treated as comment lines and are ignored.

```

#
# Parameters for Kintecus Visual Graph of Kinetic System
# (invoked with the "-chemnet:chemnet.txt" or "-chemnet" switch)
#
# All keywords are OPTIONAL and Keywords can be in any order
#
# RENDER
# Select the type of Renderer=dot[default], neato, fdp, circo, sfdp, twopi, nop, nop2, osage
render=dot
#
# TYPE
# type=species
type=species
#
# LAYOUT
# layout=topbottom, leftright [default], rightleft, bottomtop, circular
layout=topbottom
#
# Outside enclosure
# Outside=box [default], circle, oval, diamon, rounded, none
outside=rounded
#
# ARROW
# 1=reaction numbers, 2=actual line numbers [default]
ARROW=1
#
# REACTION_TYPE
# 0=just the reaction number [default], 1=prefix with character "k<number>", 2=add "k <number>"
# arrow_type=Reaction # | k | k_SPACE
Reaction_Type=k
#
# Preprocessing and Postprocessing
# pre+postprocessor(s)=0 (none), 1, 2, 3, 4 or 5
preprocessor=0
#
# FILLCOLOR
# fillcolor=black, white [default], gray, blue, red, purple, gree, yellow
fillcolor=yellow
#
# LINECOLOR
# linecolor=black[black], white, gray, blue, red, purple, green, yellow
linecolor=black
#
# SIGN
# sign= standard | flip | none | R<character_to_use> | P<character_to_use>
# standard will place a minus sign in front of reactant species names only
# and a plus, "+" in front of the reactions product's species names t
# flip : flips the signage on the reactants and products species names
# R<character> will use the single <character> in front of the reactions reactant species names
# (the product species names in the arrows with have space or nothing in front of them)
# P<character> will use the single <character> in front of the reactions prodcut species names
# (the reactant species names in the arrows with have space or nothing in front of them)
sign=flip
#
#
# Arrow_type=vectors (default) , line (none), diamond (diamond ends), circle (circle ends)
# box, curve, inv, crow, tee, vee
Arrow_type=vee
#
# Output type
# Select either png (default), jpg, gif, svg, json, ps, pdf, imap, cmmapx or fig
#
Output=jpg
#
# Combine reversible reactions into a single DOUBLE arrow
LINK=NO
#

```

Figure 20.

Again, the picture below is generated by providing the command line “-chemnet” on the Kintecus command line and using the ChemNet file as shown in the **above** figure. No additional Species Network Description file (SpecNet) has been utilized here.

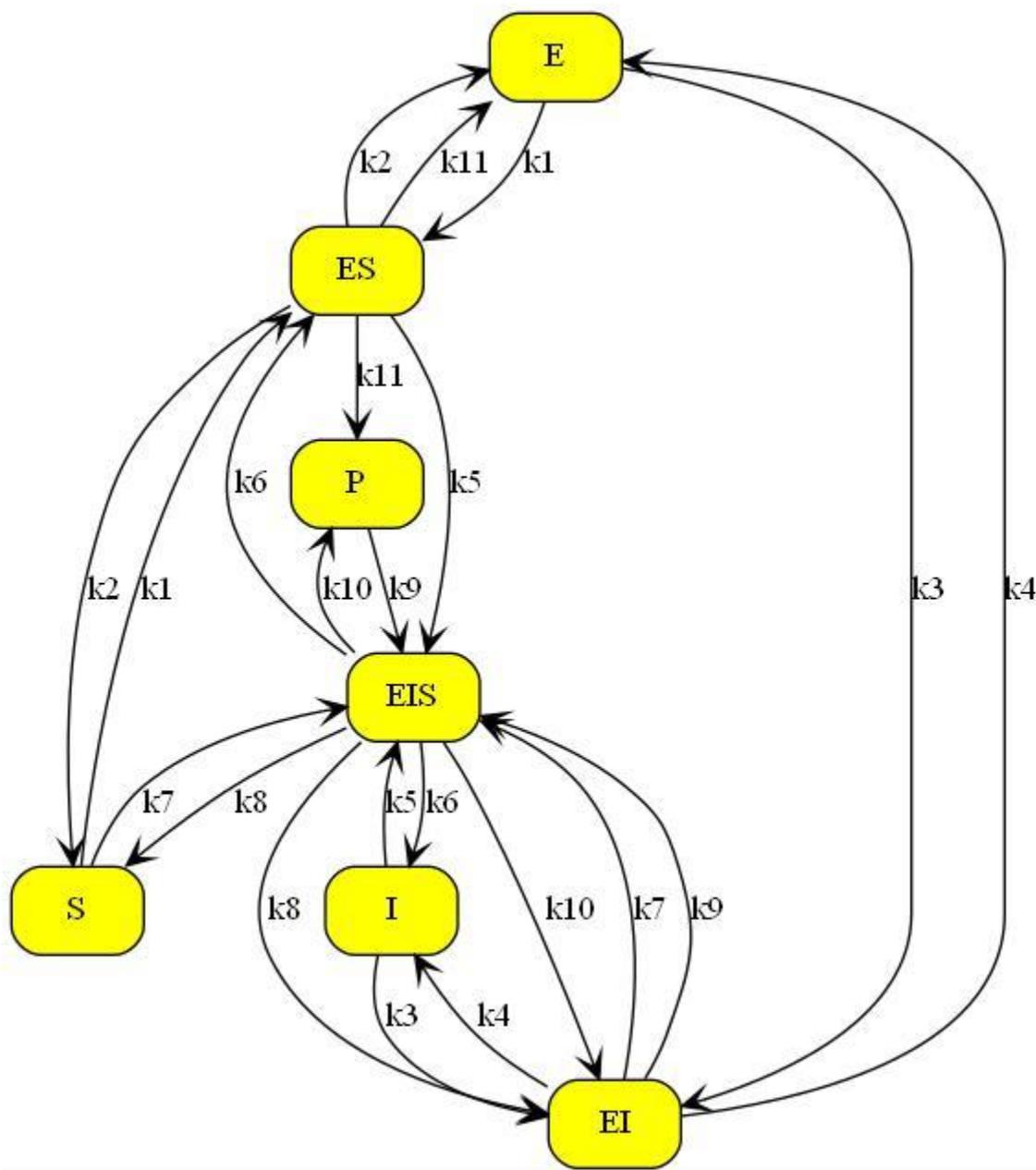


Figure 21.

To produce the picture below, change the ChemNet settings to below, and remove all Specnet settings.

Change the "LINK" keyword in the ChemNet file to "YES", "LINK=YES"

Again, there was no SpecNet file (be sure to delete the "specnet.txt" file if one is present or, it will be read in).

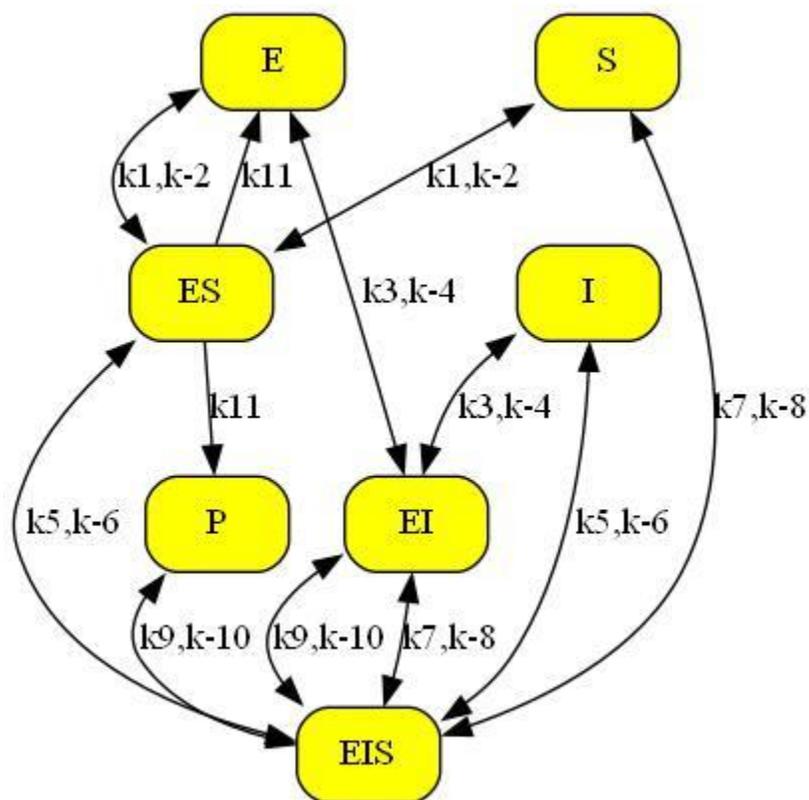


Figure 22.

To produce the picture below, change the Chemnet settings as described below.

Change the ChemNet setting "LINK" to "YES", "LINK=YES". This will combine single reaction arrows into a double reaction arrow for reactions with both a forward and reverse rate. This example is also the Kintecus-Excel file, "Chemnet\_Enzyme\_Inhibition\_Model.xlsm"

Also, a Species Description Worksheet file has been added with two entries for species, "I" and one for "S" as shown in the below table. Note that placing a "3" in the "Arrow Placement" column forces those

two species to only appear as part of a reaction arrow whether they are either a reactant or product. This is the new Specnet settings:

# Species	Arrow Placement	Display Filter	Source Color	Sink Color
# Name	(0,1,2,3)	(0,1,2,3,4,5,6)	(black, blue, red, green, gray, purple)	(black, blue, red, green, gray, purple)
# This is a sample specnet.txt input file.				
#				
# <b>Arrow Placement field values</b> == 0 Do not show as part of reaction arrow, 1 show in arrow if reactant, 2 show in arrow if product, 3 show in arrow if either reactant/product)				
#				
# <b>Display Filter</b> can take several values == 0=SHOW; 1=If reactant do not show anywhere; 2=If product do not show anywhere; 3=DO NOT SHOW AT ALL				
# 4=ONLY_SHOW_REACTANT,5=ONLY_SHOW_PRODUCT,6=ONLY_REACTANT_PRODUCT				
#				
#EIS		0	0 green	red
I		3	0 black	black
S		3	0 black	black
<b>END</b>				

And the output picture:

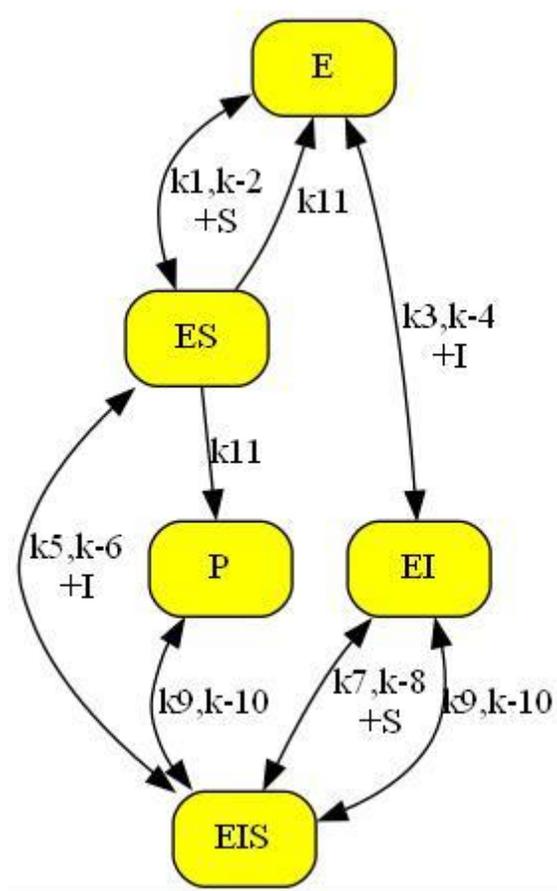


Figure 23.

Some people prefer the back-and-forth arrows but want to have the same species as part of the reaction arrow, highlight, source, and sinks. This arrangement can be accomplished by changing the LINK keyword to “No” in the ChemNet file (not shown) and using this SpecNet file:

# Species # Name	Arrow Placement (0,1,2,3)	Display Filter (0,1,2,3,4,5,6)	Source Color (black, blue, red, green, gray, purple)	Sink Color (black, blue, red, green, gray, purple)
# This is a sample specnet.txt input file.				
#				
# <b>Arrow Placement field values</b> == 0 Do not show as part of reaction arrow, 1 show in arrow if reactant, # 2 show in arrow if product, 3 show in arrow if either reactant/product)				
#				
# <b>Display Filter</b> can take several values == 0=SHOW; 1=If reactant do not show anywhere; 2=If product do not show anywhere; # 3=DO NOT SHOW AT ALL				
# 4=ONLY_SHOW_REACTANT,5=ONLY_SHOW_PRODUCT,6=ONLY_REACTANT_PRODUCT				
#				
EIS	0	0	green	red
I	3	0	black	black
S	3	0	black	black
END				

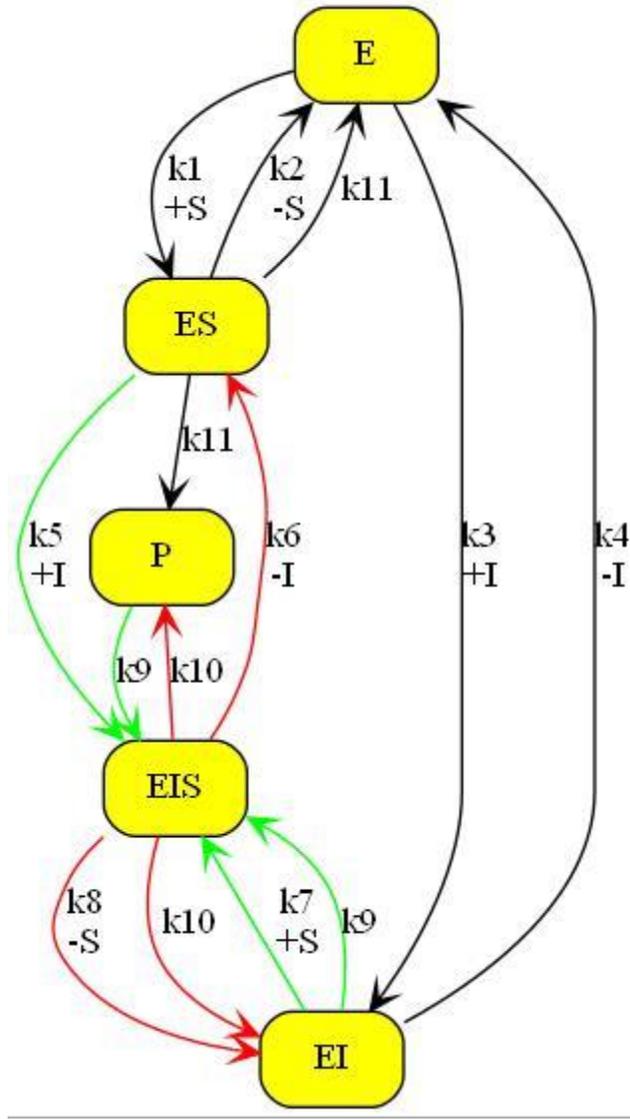


Figure 24. Note that all the sources to EIS are highlighted in green and the sinks are in red.

Note that all the sources to EIS are highlighted in green and the sinks are in red.

## Mechanism Validation with Chemnet

Kintecus can perform a full mechanism validation (by providing the “-MECHV” flag on the Kintecus Switches command line as described in the previous “Mechanism Validation” chapter) along with a Chemical Mechanism Plot will result in a chemical network mechanism plot that will highlight the four possible illegal loops (if present) in a mechanism. The illegal loops (if any are identified by “-MECHV”) will be drawn with a **dashed line** and colored in one of five colors to highlight the illegal loop.

Case	Illegal Loop Type	Illegal Loop Color
1.	Microscopic Reversibility/Rate Constant Consistency Test	Red
2.	First rho-reduction: One or more illegal irreversible loops detected	Blue
3.	Second rho-reduction: One or more illegal irreversible loops detected	Yellow
4.	Linear-Programming: One or more illegal irreversible loops detected	Purple
5.	More than one illegal loop that overlap each other	Green

The table below is generated by running the workbook “Chemnet\_Simple\_Mechanism\_Validations.xlsx” and by deleting/adding reactions for each Case described by David M. Stanbury and Dean Hoffman [2]. The table highlights the case study results (1-7) from the various valid and invalid loops present in a small, three species system as discussed in David M. Stanbury and Dean Hoffman [2]. The reaction numbers above the arrows in the pictures are the actual line numbers for the reaction as shown in the MODEL worksheet in “Chemnet\_Simple\_Mechanism\_Validations.xlsx”. This display of the actual line numbers in the reaction arrows should allow for one to follow which reactions were deleted and added for each case type discussed in [2]. The illegal loops are green because there are multiple overlapping illegal loops. The text output from Kintecus will clearly mark and explain those illegal loops. This marking of illegal loops is greatly discussed in Chapter 10, “Mechanism Validation”.

Case	Legality	Output from “-MECHV -chemnet” Kintecus command line switches
Case 1	All legal loops	
Case 2	Multiple Illegal loops	
Case 3	All legal loops	
Case 4	All legal loops	
Case 5	Multiple Illegal loops	
Case 6	Multiple Illegal loops	
Case 7	All legal loops	

The Kintecus-Excel file, "Chemnet\_Visualize\_Mechanism\_Validation\_1.xlsm" also demonstrates an illegal loop (Microscopic Reversibility/Rate Constant Consistency illegal loop) when the model in Figure 1 from Stanbury and Hoffman 2019, J.Phys Chem. [2] is run with the Kintecus Switches set to "-MECHV -chemnet" which will result in this picture showing the illegal loop as shown in Red:

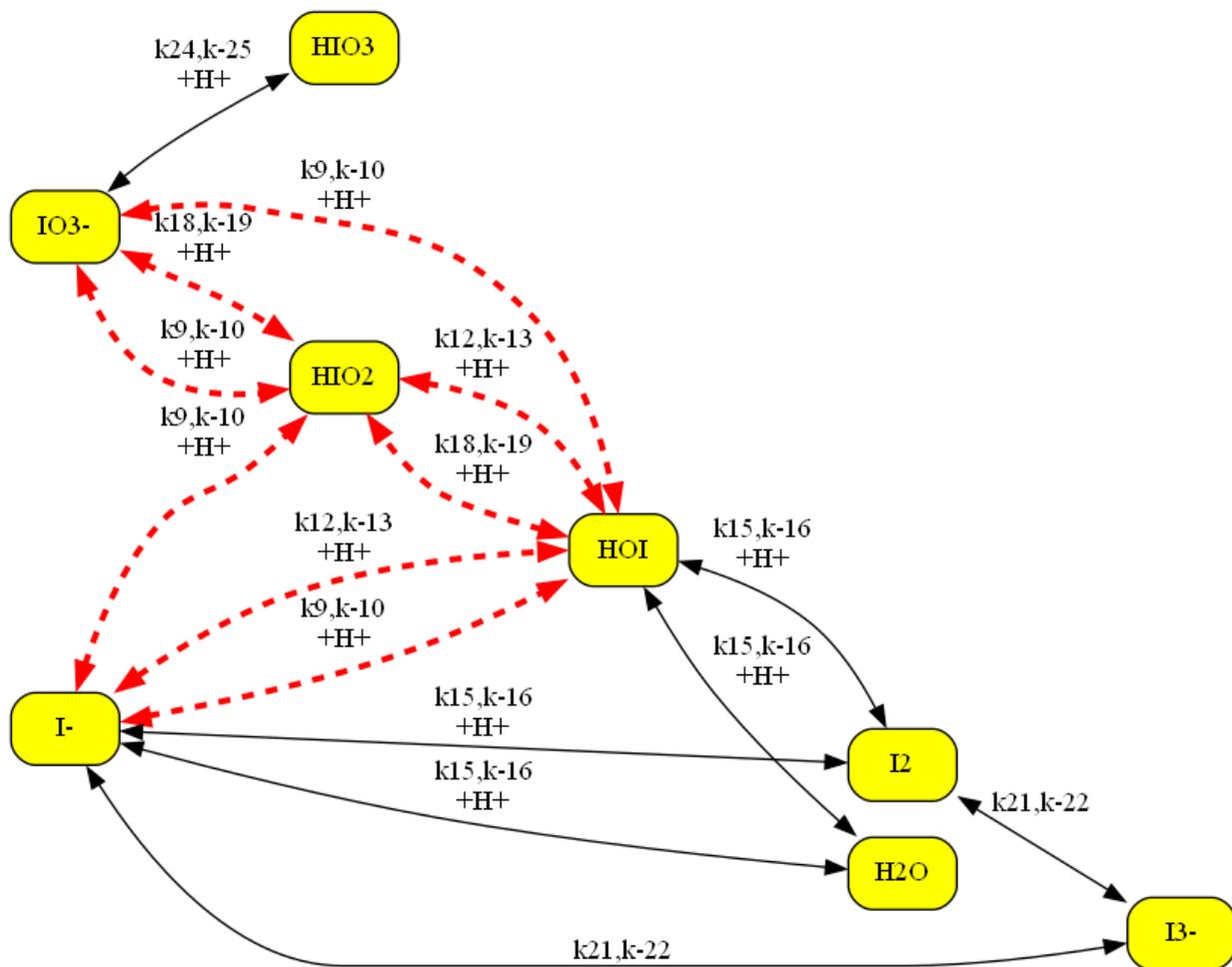


Figure 25. Using "-MECHV" (Mechanism Validation) with "-chemnet" shows illegal loops shown in figure 1, Stanbury and Hoffman 2019, J.Phys Chem. One can view the Kintecus text output for full details on this illegal loop as described in Chapter xx.

Also, the Mechanism Validation of test 4 ("Kintecus\_mechanism\_validation\_4.xls") shows illegal irreversible loops present (purple arrows) and multiple illegal overlapped loops (green arrows) as shown below:

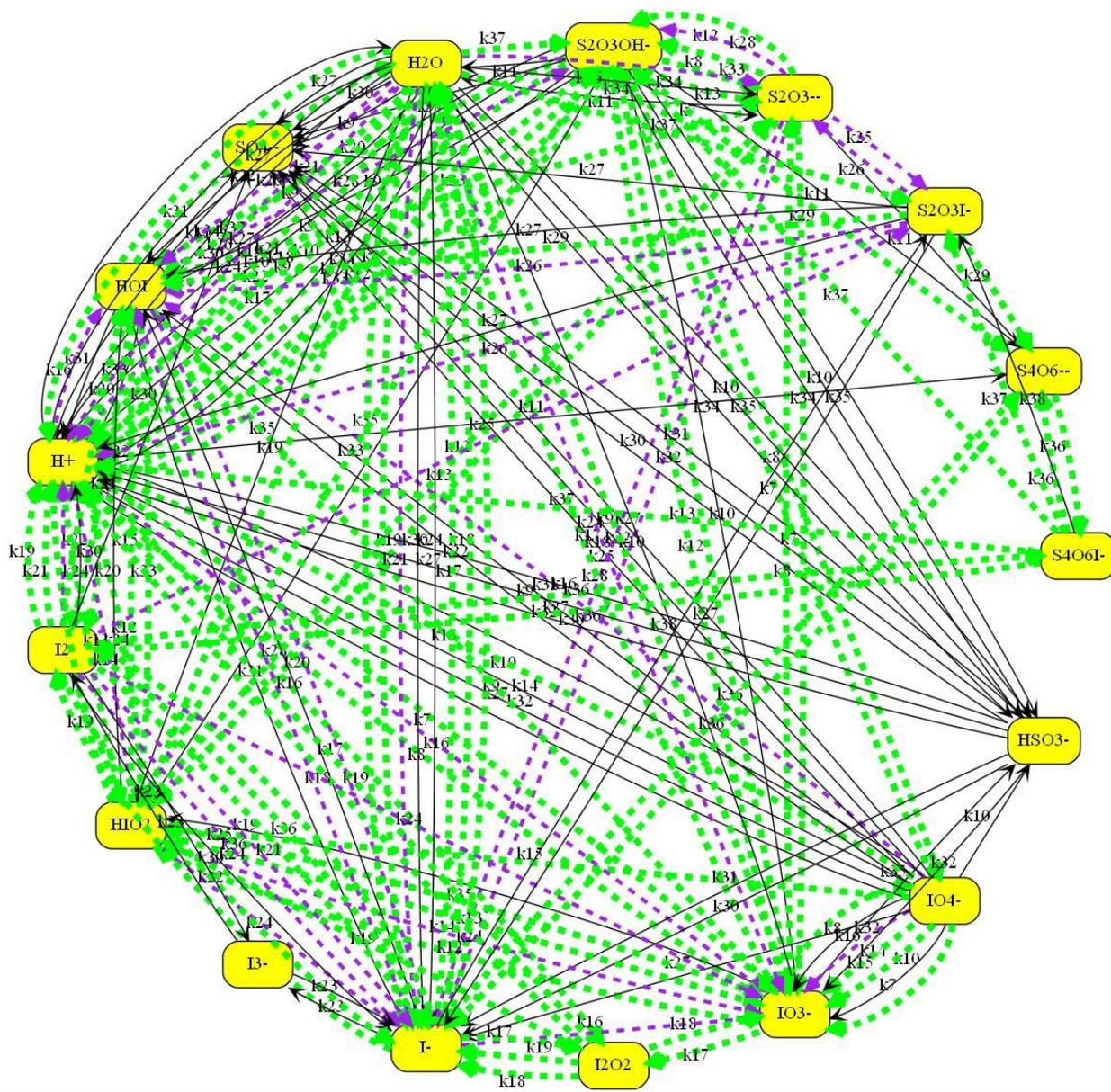
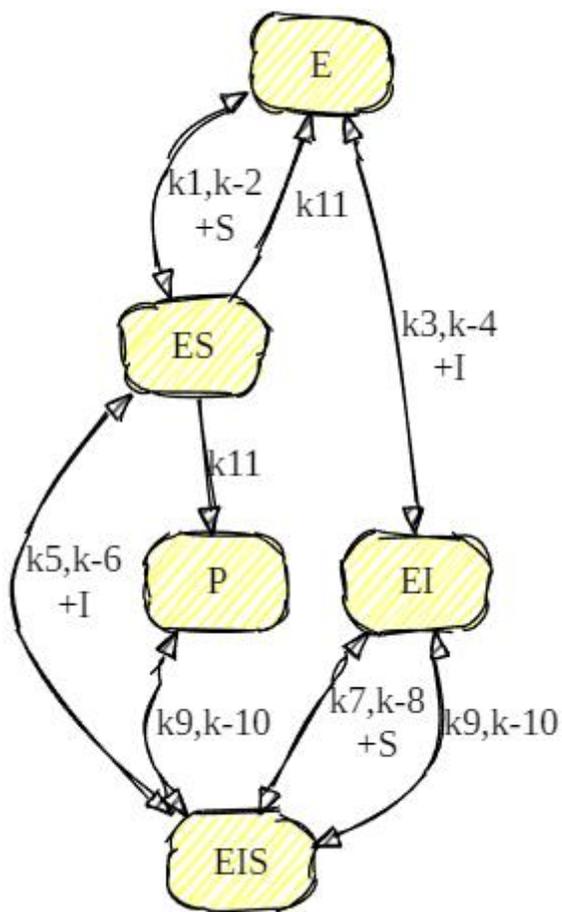


Figure 26. Using "-MECHV" (Mechanism Validation) with "-chemnet" shows illegal loops shown in figure 1, Stanbury and Hoffman 2019, J.Phys Chem. One can view the Kintecus text output for full details on this illegal loop as described in Chapter xx

## Additional Resources

Kintecus creates the graphviz text file, "chemnetout.gv" which is then read in by graphviz with various flags to output pictures and other vector drawings. The final picture or vector drawing of one's chemical mechanism may need some "fine-tuning" or editing for closer examination or better output for publication. A plethora of programs can do this and most are described at [www.graphviz.org/resources](http://www.graphviz.org/resources). Also, some external programs can further analyze one's mechanism, such as "Gephi" at "gephi.org," and for publication output, one can save or output files as "SVG" files for use in "PGF/Tikz" or "dot2tex" or "inkscape.org". One can even emulate "hand-sketches" of your models by inputting the gv file into "sketchviz" at "sketchviz.org" :



## I Don't Where to Start!

One needs to provide the "-chemnet" flag on the Kintecus command line and run Kintecus. That's it. A default picture of your chemical mechanism named, "chemnetwork.jpg" will be output where Kintecus is stored (usually "C:\Kintecus\", so your picture will be in "C:\Kintecus\chemnetwork.jpg"). It will be in boring black and white. If you want to add more color and display reaction numbers on the arrows, copy the "O\_Chemnet.txt" worksheet from an existing Kintecus-Excel file such as "chemnet\_Enzyme\_Inhibition\_Model.xlsm" or "Chemnet\_sample1\_Pires and Faria Inorg Chem 2021 photochemical chloration-iodide clock reaction.xlsm" and many others.

## References:

[1] Graphviz by John Ellson (drivers and plugins, scripting and codegen extensions, build), Emden Gansner (dot, neato, twopi, circo, fdp, osage, smyrna, gvmap, prism, gvpr), Yifan Hu (sfdp, prism, gvmap, cluster, mm2gv), Stephen North (dot, neato) and many others (see [www.graphviz.org/credits/](http://www.graphviz.org/credits/) )

[2] David M. Stanbury and Dean Hoffman; "Systematic Application of the Principle of Detailed Balancing to Complex Homogeneous Chemical Reaction Mechanisms"; J. Phys. Chem A; 2019; 123, p5436-5445 and references therein. (a) Wegscheider, R. Über simultane Gleichgewichte und die Beziehungen zwischen Thermodynamik und Reaktionskinetik homogener Systeme. Monatsh. Chem. 1901, 22, 849–906 (b) Wegscheider, R. Über simultane Gleichgewichte die Beziehung