# Next Generation Integrated Simulation Platform to Cover All Engineering Phases of $CO_2$ Power Cycle

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# Next Generation Integrated $CO_2$ Power Cycle Simulation

> Agenda

1. Objectives
2. Measures to Achieve Objectives
3. Introducing SimCentral®
4. Conclusions

# Engineering Life Cycle for $CO_2$ Power Cycle Plants

> Background: Actual and practical utilization of $CO_2$ Power Cycles requires completing all of the engineering steps based not only on steady-state simulation but also dynamic simulation incorporating detailed mechanical information and control strategy.

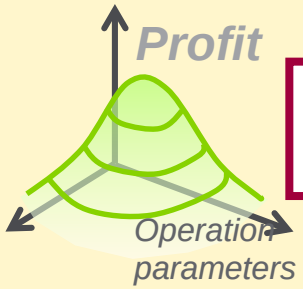
- **Basic Design**: Steady-state heat and material balance is calculated under specified conditions such as load and temperature of heat source. Perform rough equipment sizing.
- **Detail Design**: After sizing and selecting equipment, steady-state simulation is done again to know “actual” operating conditions. Dynamic simulation establishes the control logic and operating manual.
- **Operational Analysis**: By comparing actual operation with simulation, various parameters can be determined such as efficiency of each compressor, or expanders, and heat exchangers.

# Objectives

> Conventional approaches require multiple software products and a tedious manual integration procedure.

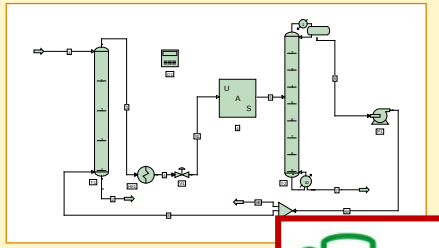
> A new integrated simulation platform can serve all of the engineering phases with highly accurate, reliable and robust simulation capability, to save significant time and cost all through the plant lifecycle.

## Optimization tool



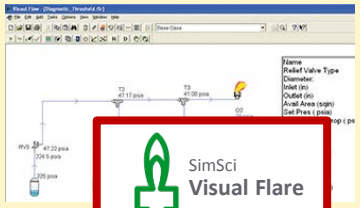

SimSci ROMeo

## Steady state simulator



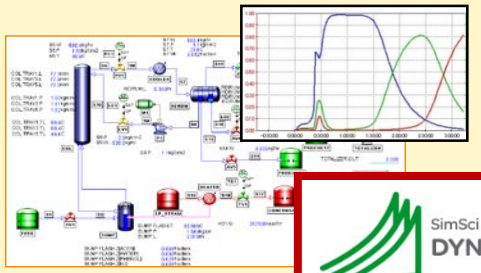
SimSci PRO/II


## Fluid Flow simulator



SimSci Visual Flare

## Dynamic simulator



SimSci DYNSIM

**Accurate thermodynamic methods**

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# Measures to Achieve Objectives

> Establish a novel and integrated simulation platform utilizing modern ease of use, multiple simulation modes, and custom modeling.

> Equip the platform with highly accurate Wagner Equation of State (EOS) for $CO_2$.

# Span and Wagner Equation of State

> Outline of the EOS [1)]

$$\phi(\delta,\tau)=\phi^{o}(\delta,\tau)+\phi^{r}(\delta,\tau),$$

$$\phi^{r}=\sum_{i=1}^{7} n_i\delta^{d_i}\tau^{t_i}+\sum_{i=8}^{34} n_i\delta^{d_i}\tau^{t_i}e^{-\delta^{c_i}}$$

$$+\sum_{i=35}^{39} n_i\delta^{d_i}\tau^{t_i}e^{-\alpha_i(\delta-\epsilon_i)^2-\beta_i(\tau-\gamma_i)^2}$$

$$+\sum_{i=40}^{42} n_i\Delta^{b_i}\delta\, e^{-C_i(\delta-1)^2-D_i(\tau-1)^2}$$

$$\text{with}\quad \Delta=\{(1-\tau)+A_i[(\delta-1)^2]^{1/(2\beta_i)}\}^2+B_i[(\delta-1)^2]^{a_i}.$$

| $i$ | $n_i$ | $d_i$ | $t_i$ |
|---|---|---|---|
| 1 | 0.388 568 232 031 61×10^0 | 1 | 0.00 |
| 2 | 0.293 854 759 427 40×10^1 | 1 | 0.75 |
| 3 | −0.558 671 885 349 34×10^1 | 1 | 1.00 |
| 4 | −0.767 531 995 924 77×10^0 | 1 | 2.00 |
| 5 | 0.317 290 055 804 16×10^0 | 2 | 0.75 |
| 6 | 0.548 033 158 977 67×10^0 | 2 | 2.00 |
| 7 | 0.122 794 112 203 35×10^0 | 3 | 0.75 |

| $i$ | $n_i$ | $d_i$ | $t_i$ | $c_i$ |
|---|---|---|---|---|
| 8 | 0.216 589 615 432 20×10^1 | 1 | 1.50 | 1 |
| 9 | 0.158 417 351 097 24×10^1 | 2 | 1.50 | 1 |
| 10 | −0.231 327 054 055 03×10^0 | 4 | 2.50 | 1 |
| 11 | 0.581 169 164 314 36×10^−1 | 5 | 0.00 | 1 |
| 12 | −0.553 691 372 053 82×10^0 | 5 | 1.50 | 1 |
| 13 | 0.489 466 159 094 22×10^0 | 5 | 2.00 | 1 |
| 14 | −0.242 757 398 435 01×10^−1 | 6 | 0.00 | 1 |
| 15 | 0.624 947 905 016 78×10^−1 | 6 | 1.00 | 1 |
| 16 | −0.121 758 602 252 46×10^0 | 6 | 2.00 | 1 |
| 17 | −0.370 556 852 700 86×10^0 | 1 | 3.00 | 2 |
| 18 | −0.167 758 797 004 26×10^−1 | 1 | 6.00 | 2 |
| 19 | −0.119 607 366 379 87×10^0 | 4 | 3.00 | 2 |
| 20 | −0.456 193 625 087 78×10^−1 | 4 | 6.00 | 2 |
| 21 | 0.356 127 892 703 46×10^−1 | 4 | 8.00 | 2 |
| 22 | −0.744 277 271 320 52×10^−2 | 7 | 6.00 | 2 |
| 23 | −0.173 957 049 024 32×10^−2 | 8 | 0.00 | 2 |
| 24 | −0.218 101 212 895 27×10^−1 | 2 | 7.00 | 3 |
| 25 | 0.243 321 665 592 36×10^−1 | 3 | 12.00 | 3 |
| 26 | −0.374 401 334 234 63×10^−1 | 3 | 16.00 | 3 |
| 27 | 0.143 387 157 568 78×10^0 | 5 | 22.00 | 4 |
| 28 | −0.134 919 690 832 86×10^0 | 5 | 24.00 | 4 |
| 29 | −0.231 512 250 534 80×10^−1 | 6 | 16.00 | 4 |
| 30 | 0.123 631 254 929 01×10^−1 | 7 | 24.00 | 4 |
| 31 | 0.210 583 219 729 40×10^−2 | 8 | 8.00 | 4 |
| 32 | −0.339 585 190 263 68×10^−3 | 10 | 2.00 | 4 |
| 33 | 0.559 936 517 715 92×10^−2 | 4 | 28.00 | 5 |
| 34 | −0.303 351 180 556 46×10^−3 | 8 | 14.00 | 6 |

| $i$ | $n_i$ | $d_i$ | $t_i$ | $\alpha_i$ | $\beta_i$ | $\gamma_i$ | $\epsilon_i$ |
|---|---|---|---|---|---|---|---|
| 35 | −0.213 654 886 883 20×10^3 | 2 | 1.00 | 25 | 325 | 1.16 | 1.00 |
| 36 | 0.266 415 691 492 72×10^5 | 2 | 0.00 | 25 | 300 | 1.19 | 1.00 |
| 37 | −0.240 272 122 045 57×10^5 | 2 | 1.00 | 25 | 300 | 1.19 | 1.00 |
| 38 | −0.283 416 034 239 99×10^3 | 3 | 3.00 | 15 | 275 | 1.25 | 1.00 |
| 39 | 0.212 472 844 001 79×10^3 | 3 | 3.00 | 20 | 275 | 1.22 | 1.00 |

| $i$ | $n_i$ | $a_i$ | $b_i$ | $\beta_i$ | $A_i$ | $B_i$ | $C_i$ | $D_i$ |
|---|---|---|---|---|---|---|---|---|
| 40 | −0.666 422 765 407 51×10^0 | 3.500 | 0.875 | 0.300 | 0.700 | 0.3 | 10.0 | 275 |
| 41 | 0.726 086 323 498 97×10^0 | 3.500 | 0.925 | 0.300 | 0.700 | 0.3 | 10.0 | 275 |
| 42 | 0.550 686 686 128 42×10^−1 | 3.000 | 0.875 | 0.300 | 0.700 | 1.0 | 12.5 | 275 |

[a] $R = 0.188\,924\,1$ kJ/(kg K); $T_c = 304.128\,2$ K; $\rho_c = 467.6$ kg/m$^3$.

1) Span,R. and Wagner W.; “A New Equation of State for Carbon Dioxide Covering Fluid Region from Triple Point Temperature to 1100K at Pressure up to 800MPa”, J.Phys.Chem.Ref.Data,25(6), 1509-1596 (1996)

# Span and Wagner Equation of State

> Highly accurate to cover supercritical $CO_2$

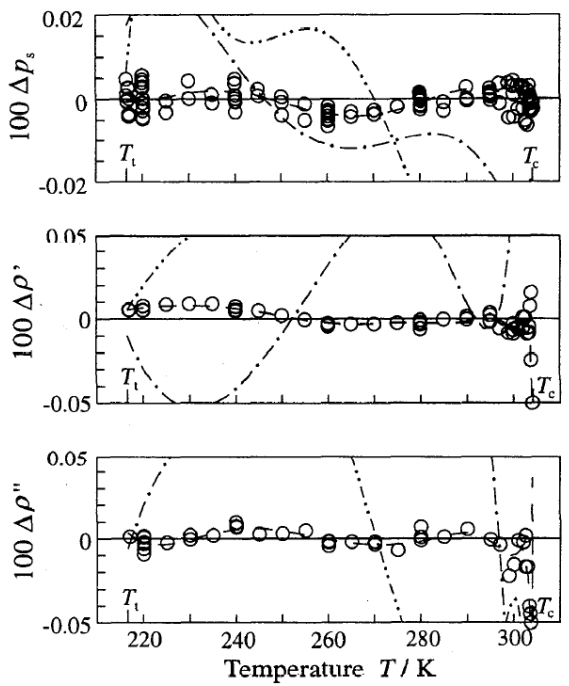


FIG. 18. Relative deviations $100\Delta y = 100\ (y_{exp} - y_{calc})/y_{exp}(y = p_s, \rho', \rho'')$ of the experimental saturation data of Duschek *et al.*[58] from values calculated from Eq. (6.1). Values calculated from auxiliary equations presented in Sec. 3, the equation of state of Ely *et al.*[15] and the auxiliary equations of Angus *et al.*[3] are plotted for comparison.

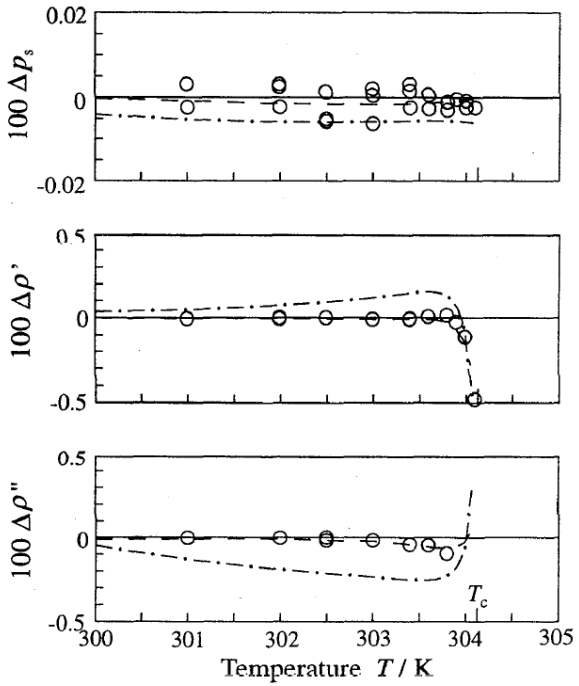


FIG. 19. Relative deviations $100\Delta y = 100\ (y_{exp} - y_{calc})/y_{exp}$ $(y = p_s, \rho', \rho'')$ of the near critical experimental saturation data of Duschek *et al.*[58] from values calculated from Eq. (6.1). Values calculated from the auxiliary equations presented in Sec. 3 and from the crossover of Chen *et al.*[27] are plotted for comparison.

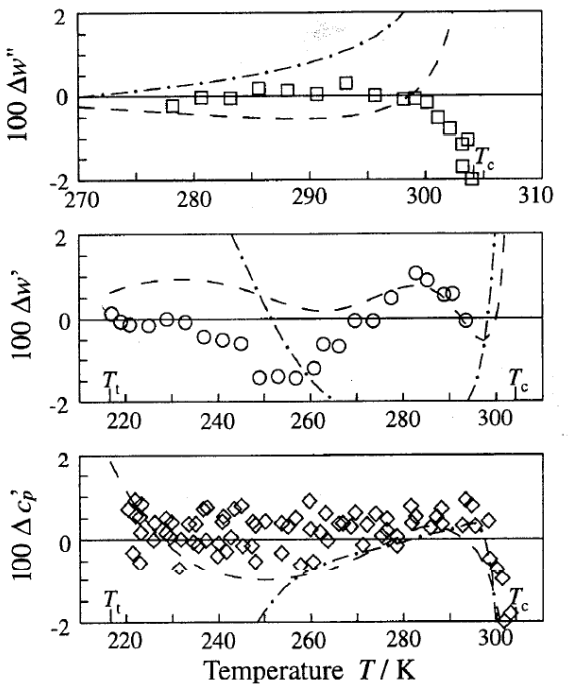


FIG. 20. Relative deviations $100\Delta y = 100\ (y_{exp} - y_{calc})/y_{exp}$ $(y = w'', w', c_p')$ of experimental caloric data at saturation from values calculated from Eq. (6.1). Data calculated from the wide-range equations of Ely *et al.*[15] and Angus *et al.*[3] are plotted for comparison.

Source: Span,R. and Wagner W.; "A New Equation of State for Carbon Dioxide Covering Fluid Region from Triple Point Temperature to 1100K at Pressure up to 800MPa", J.Phys.Chem.Ref.Data,25(6),1509-1596 (1996)

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# Introducing SimCentral®

> A new Simulation Platform is being developed using a newly-devised mathematical framework for solving large sets of non-linear simultaneous equations based on multi-core CPU technology.

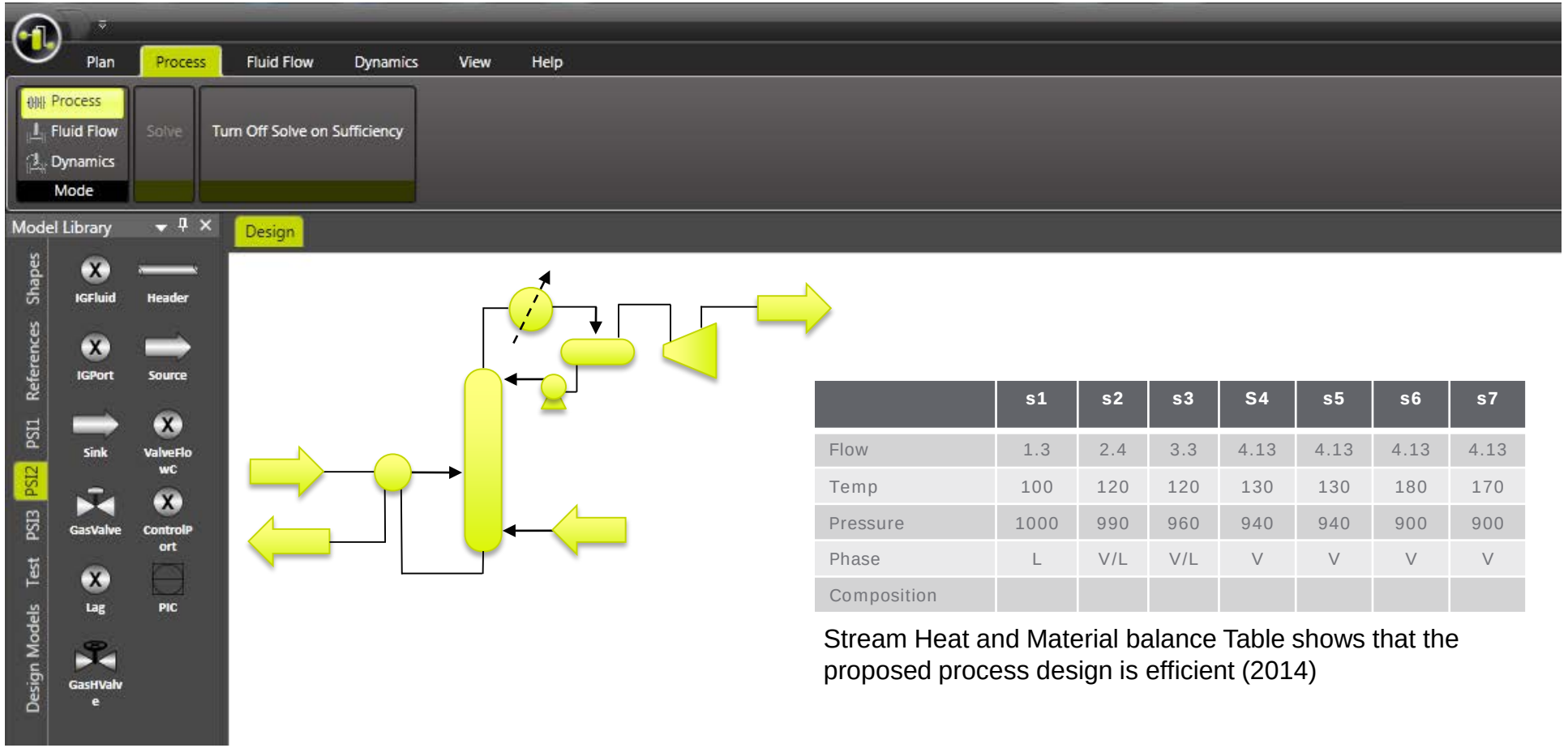
> Wagner EOS was incorporated into the platform to predict thermodynamic properties of $CO_2$.

> Successfully created steady state demonstration of a $CO_2$ Power Cycle.

> The simulation converts to a dynamic simulation for future control analysis.

# Introducing SimCentral®

- > Process mode
  - > Steady state simulation using a sophisticated equation solver.

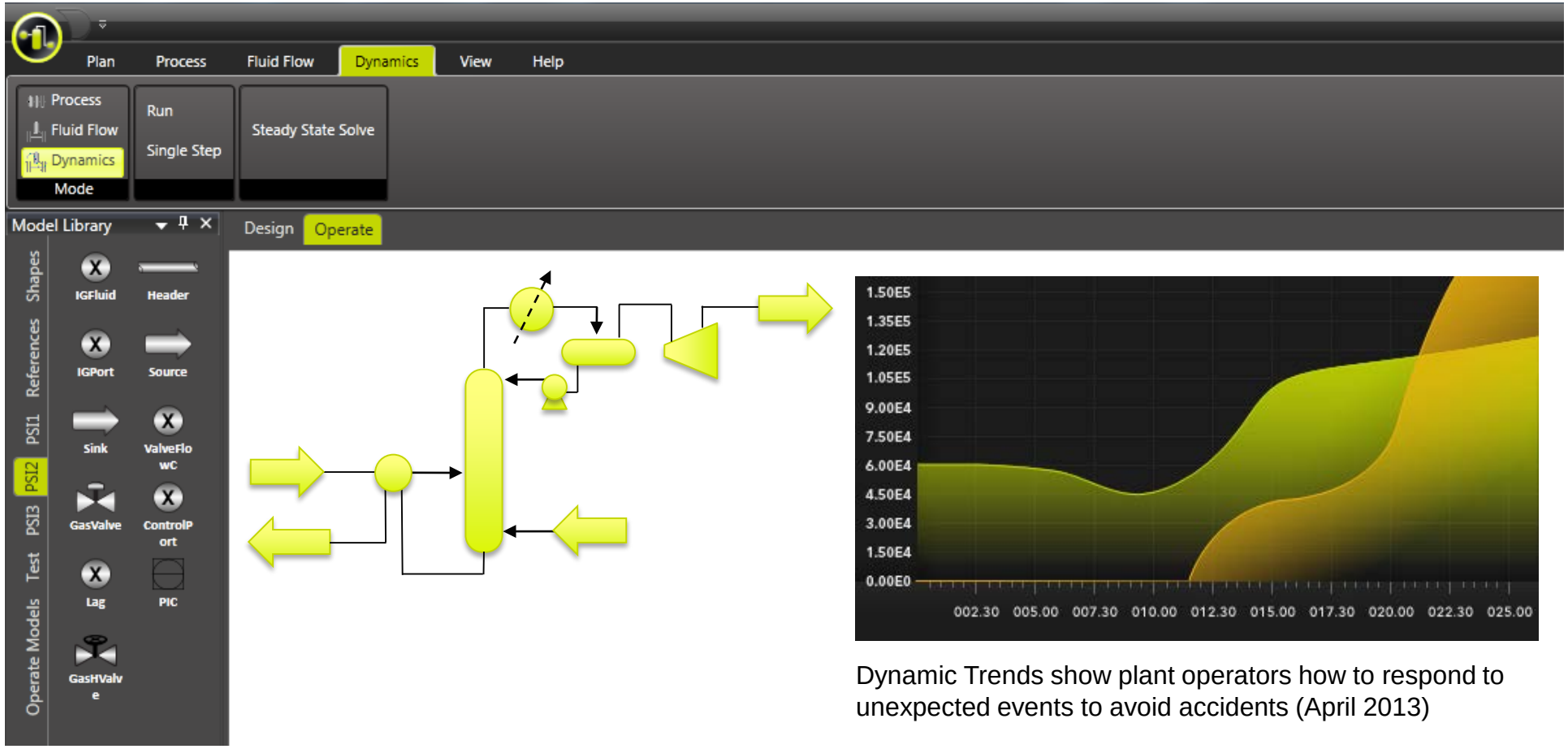



| | s1 | s2 | s3 | S4 | s5 | s6 | s7 |
|---|---|---|---|---|---|---|---|
| Flow | 1.3 | 2.4 | 3.3 | 4.13 | 4.13 | 4.13 | 4.13 |
| Temp | 100 | 120 | 120 | 130 | 130 | 180 | 170 |
| Pressure | 1000 | 990 | 960 | 940 | 940 | 900 | 900 |
| Phase | L | V/L | V/L | V | V | V | V |
| Composition | | | | | | | |

Stream Heat and Material balance Table shows that the proposed process design is efficient (2014)

# Introducing SimCentral®

- > Dynamic mode
  - > Dynamic simulation (using same model created in Process mode)




Dynamic Trends show plant operators how to respond to unexpected events to avoid accidents (April 2013)

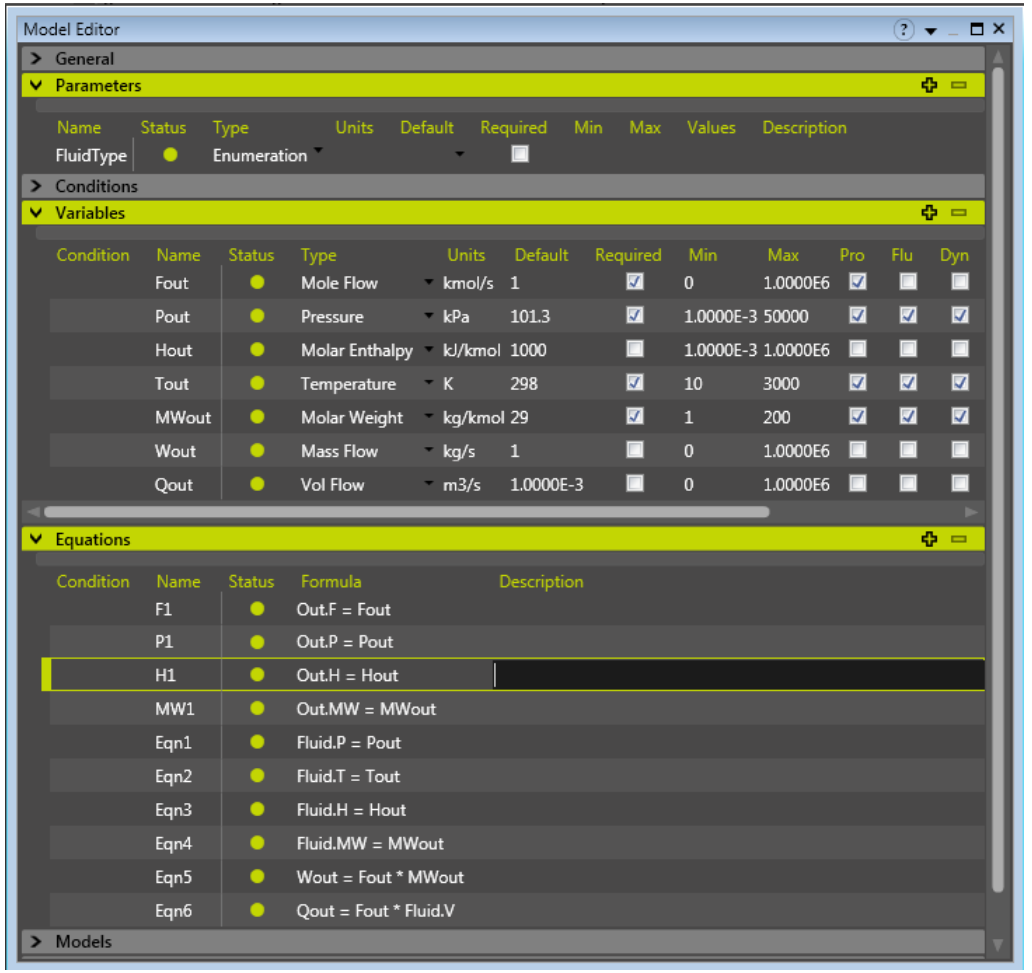
# Introducing SimCentral®

> Multi-user Collaboration:
  > Shared Simulation Repository
  > Multi-client  and Cloud-ready

# Introducing SimCentral®

> Ready to incorporate user-defined models
  > No need for software coding
  > Define variables
    - Units of Measure
    - Default Specification
    - Default value
    - Required Input Flag
  > Define Equations
    - Free form input like (example heat balance)

    $F_{in,1}*h_{in,1}+F_{in,2}h_{in,2}=F_{out}h_{out}$
  > Subnodes



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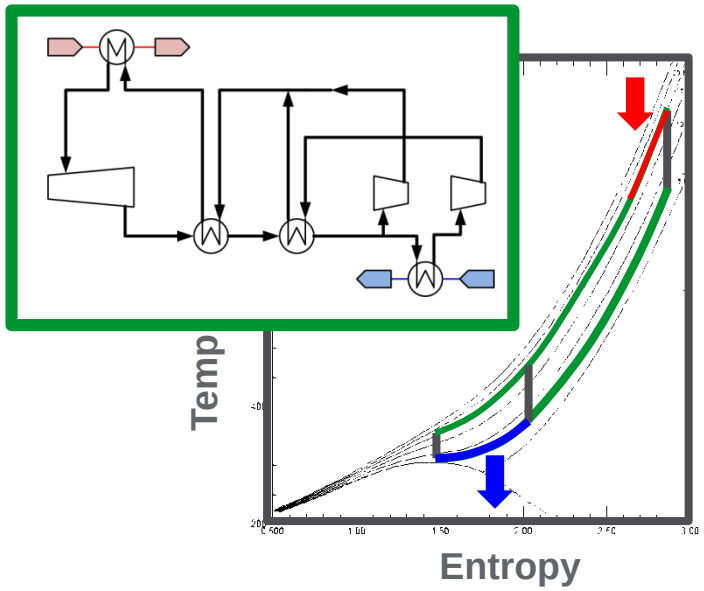
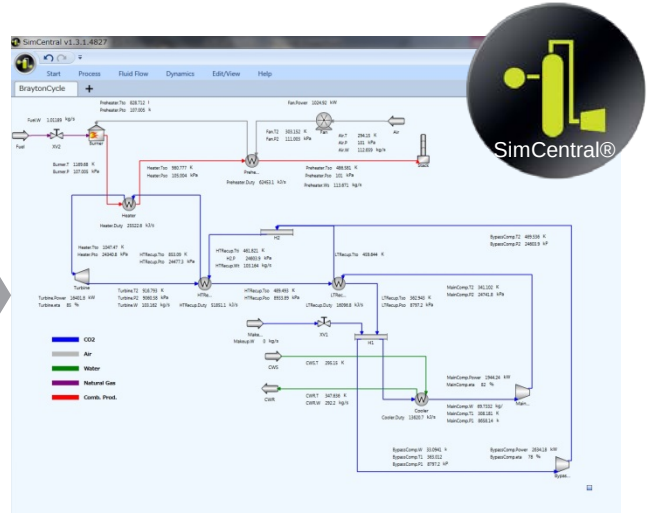
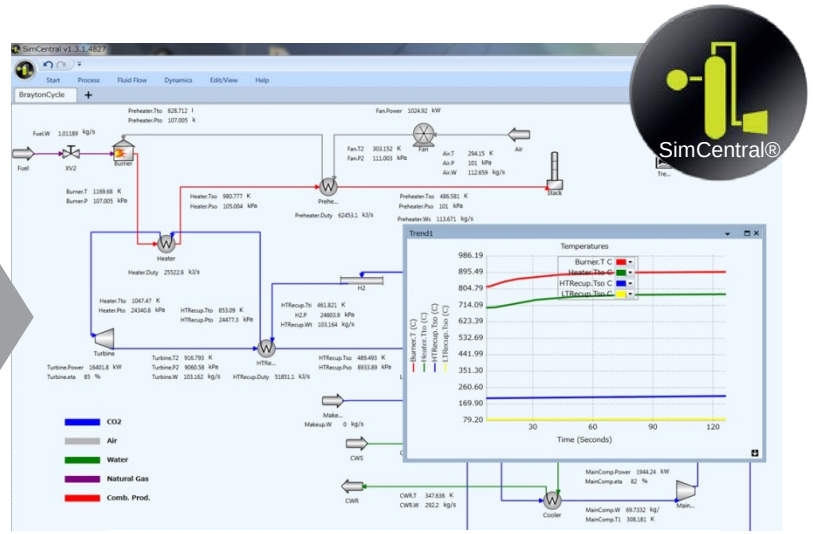
# SimCentral Benchmark Example

> Process based on literatures like Yoonhan Ahn et al.[2)]
> Circulating rate of $CO_2$ was readily determined in consistent “degree of freedom”.
> Successfully converts to dynamic model, incorporating mechanical data such as response time of actuator and shaft inertia of the compressors and the turbine.




Steady-state solution on SimCentral using **Wagner-EOS**




Dynamic solution
(switch to dynamic mode)

2) Yoonhan Ahn, Jeong Ik Lee et al. “Review of Supercritical CO2 Power Cycle Technology and Current Status of Research and Development “, Nucl Eng Technolol 47, 647-661 (2015)

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# Conclusions

> This work has established a single and integrated simulation platform which is rigorous, accurate, robust, and fast; it can be applied to all the engineering phases of $CO_2$ Power Cycle design. On the platform we can;
  > Convert steady state model to dynamic model
  > Multiple-users can access a model
  > Make the most of cloud features

> Wagner's accurate equations of state was incorporated.

> Example model was successfully created to demonstrate that the process configuration can be optimized using the simulation model.

Come see our poster!

# Thank you!

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