SMILE - A Modern Process Simulation Framework – Numerical Solution Strategies and Physical Properties
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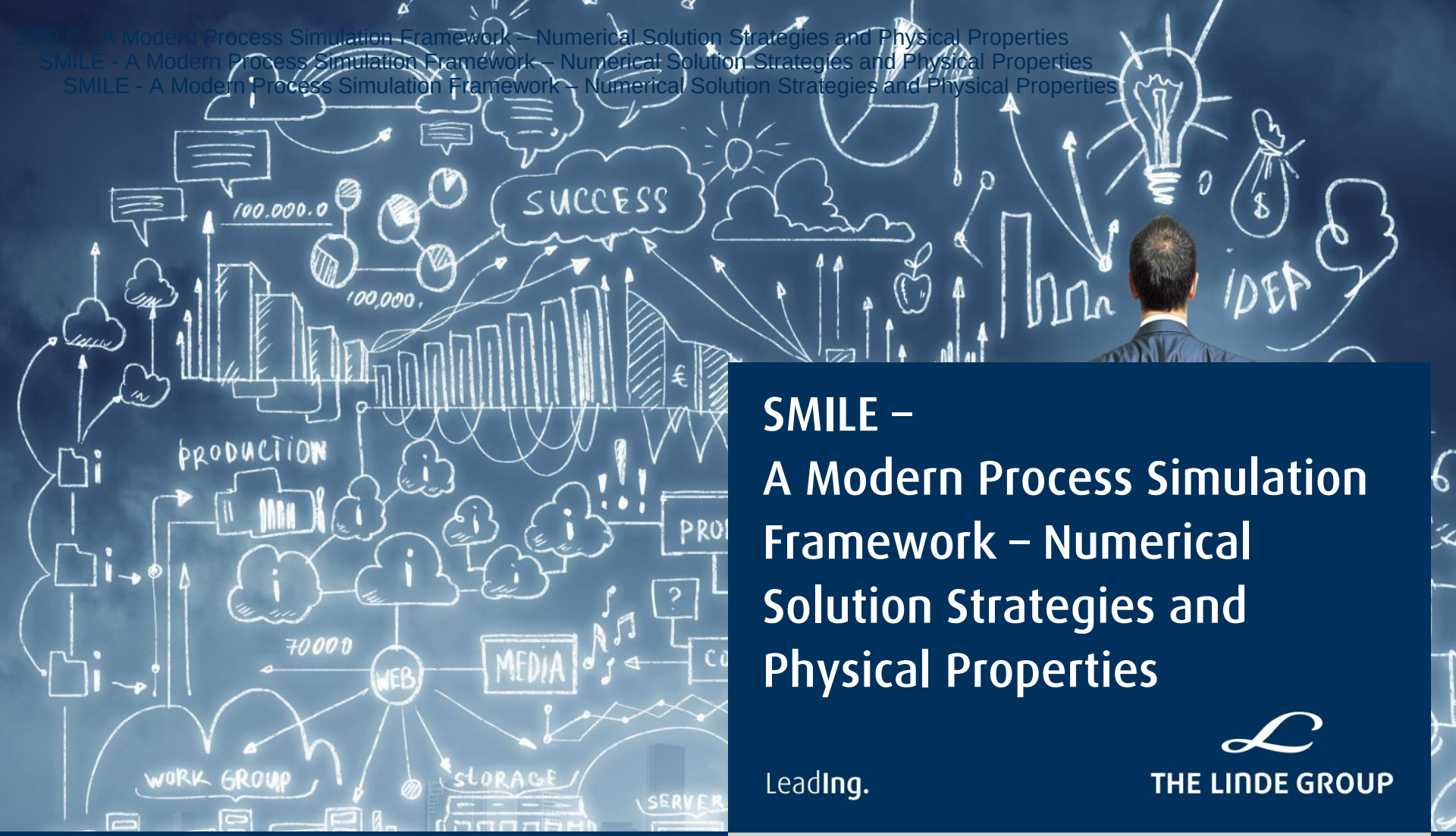

SMILE – A Modern Process Simulation Framework – Numerical Solution Strategies and Physical Properties

LeadIng.

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Munich, July, 2020

Driving forces for Dev of Process Simulation @ Linde Engineering

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- **Integration of Workflows Process Design <-> Eq Design <-> Cost Estimation <-> Safety <-> Control**
- **Ever Increasing Depth of Equipment Models =>**
  - Increasing complexity of Software Engineering and numerics
  - Modular Hierarchic Modeling, enhanced collaboration IT <-> Engng in Software Dev
  - Reduce complexity of Software Dev (FORTRAN -> python, AD, modeling languages)
- **(Increasingly) Heterogeneous environment w.r.t. Software and Operating System (UNISIM, OPTISIM, python, Docker, web APIs)**
  - Software standards and portable tools become more improtant
- **New applications such as NMPC, online optimization, health monitoring**

- **Enhanced Scope of Applicability of Process / Eq Simulations – modeling extremal scenarips such as start up, shut down (for innovative control strategies)**
  - Pressure driven flow

- **=> SMILE (2014 -)**

A recent survey regarding the process industry's usage and requirements regarding simulation tools and methods

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The Role of Simulation within the Life-Cycle of a Process Plant

Results of a global online survey

Mathias Oppelt, Prof. Dr. Mike Barth and Prof. Dr. Leon Urbas
Siemens AG, Hochschule Pforzheim, Technische Universität Dresde

"System integrators are in strong need for process models, simulation libraries, **modeling standards** and **open interfaces**." (S31)

"Equipment manufacturers will provide simulation models for their equipment in the future. " (S32)

- **How is simulation used along the life cycle of a process plant today?**
- **What is the common vision about the future use of simulation?**
- **How can this vision be reached?**

"Investigating statements about the future (Figure 25) indicated that an important functionality to enable a continuous use of simulation across the life-cycle of a process plant is **a modular, flexible and open** tool landscape."

"**Integrated engineering**, simulation and **standards** are the most relevant technological trends that will change the way we work." (S 26)

SMILE provides a comprehensive scriptable work bench for modeling & simulation

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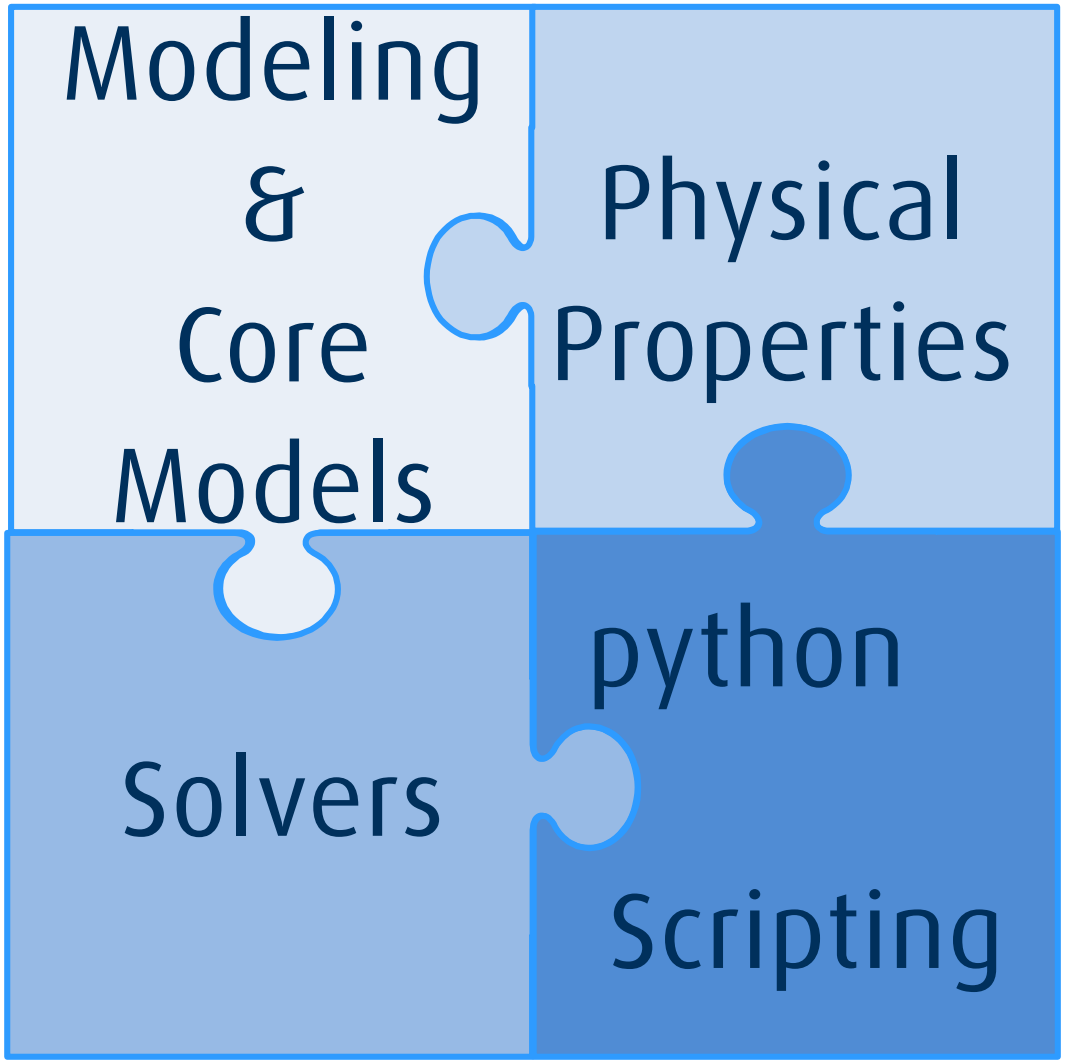
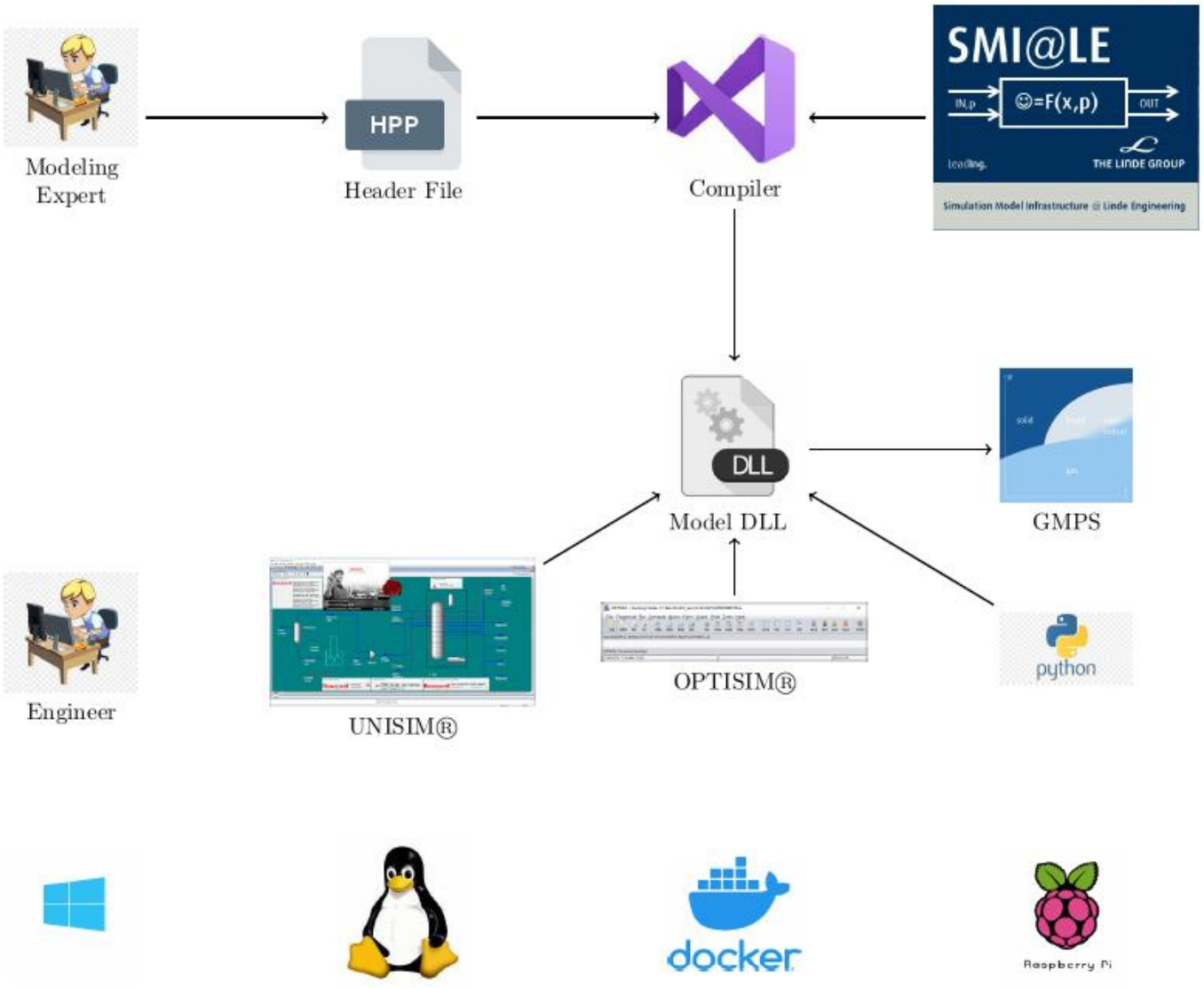
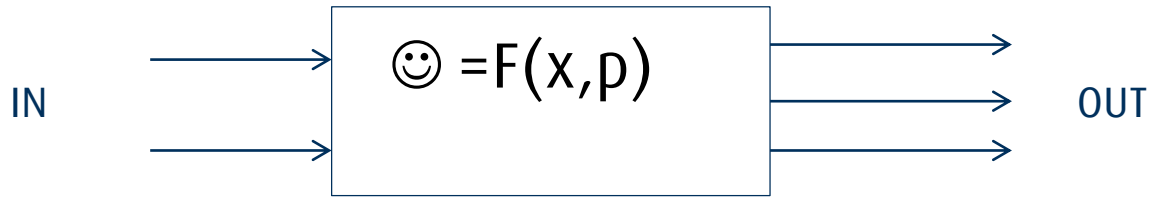


Practical Setup for SMILE Model development: A user model is compiled using "SMILE Redistributable" into DLL



What is a SMILE Model?



A SMILE Model...

- is a (Black, White or Grey Box) mathematical model of a technical or physical system, e.g. of a process or a process unit
- has Inputs and Outputs
- Math POV: Model is typically a a function, an ODE, an equation system, DAE, BVP or optimization problem (but may be something else)
- IT POV: DLL (or shared library) that may be used in a variety of systems, i.e. from OPTISIM® , UNISIM®, python, Excel, C/C++, Fortran, ...

Requirements regarding Physical Property from SMILE applications – 1 –

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- Fast (-> native software interfaces, native DLL or comparable fast)
- Multi threading, 64 bit, portable code, python bindings
- Different choices for independent variables

$$\rho(z,T,p),\ \rho(z,h,p),\ \rho(z,u,v),\ \rho(z,s,p)$$

- Derivatives for all independent quantities, i.e.

$$\frac{\partial\rho(z,T,p)}{\partial z_j},\ \frac{\partial\rho(z,T,p)}{\partial T},\ \frac{\partial\rho(z,T,p)}{\partial p},\ldots$$

- Builk derivatves, i.e.
  - Assume that Stream has a Vapour and Liquid Phase. Then, the partial derivative should return the derivatives of the bulk based on correct mixing rules
- Means for Debugging:
  - Optional throwing of Exceptions for non-physical states (p<0)
  - Extensive, configurable logging

Requirements regarding Physical Property from SMILE applications – 2 –

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- Optional usage of quadruple precision
- Method for explicit multi-phase flash:

$$(z_j, T, p) \mapsto x_j, y_j, z_j, \ldots$$

- Ideally: open source basis implementation providing basic equations of state, more sophisticated methods are proprietary
- Software component representing of flash result to obtain different properties (vf, x, y) w/o repeating flash calculation

SMILE Models are often set up in hierarchical manner

Example: HEX is combination of Metals, alpha, flow passage models

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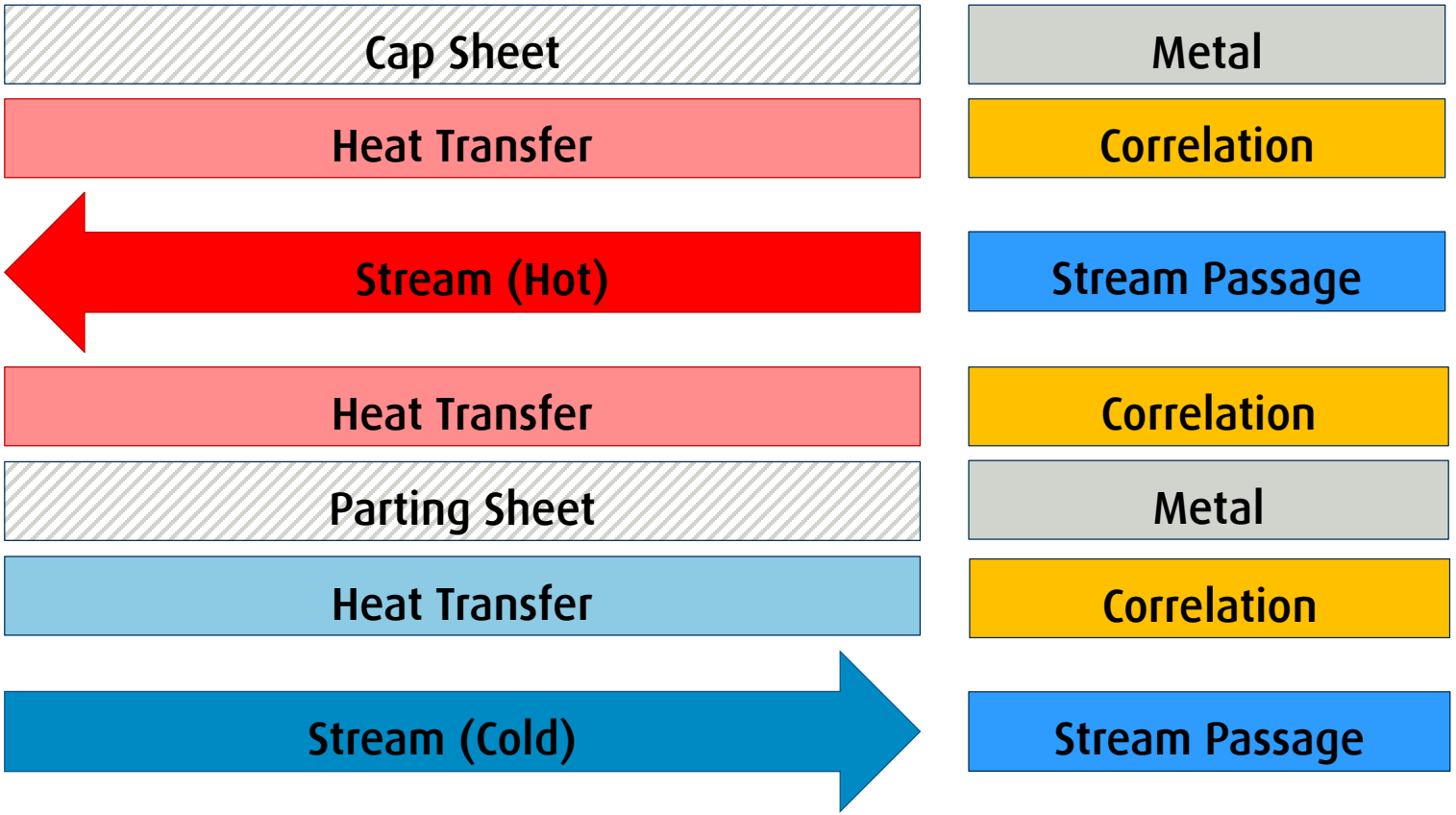
Plate Fin Heat Exchangers – Advanced Topology

- Streams separated by parting sheets
- Boundary: Cap Sheets



SWHE re-uses same models and replaces only alpha model

Base Units

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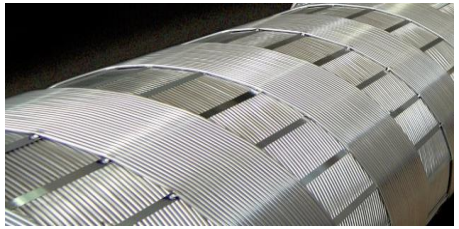
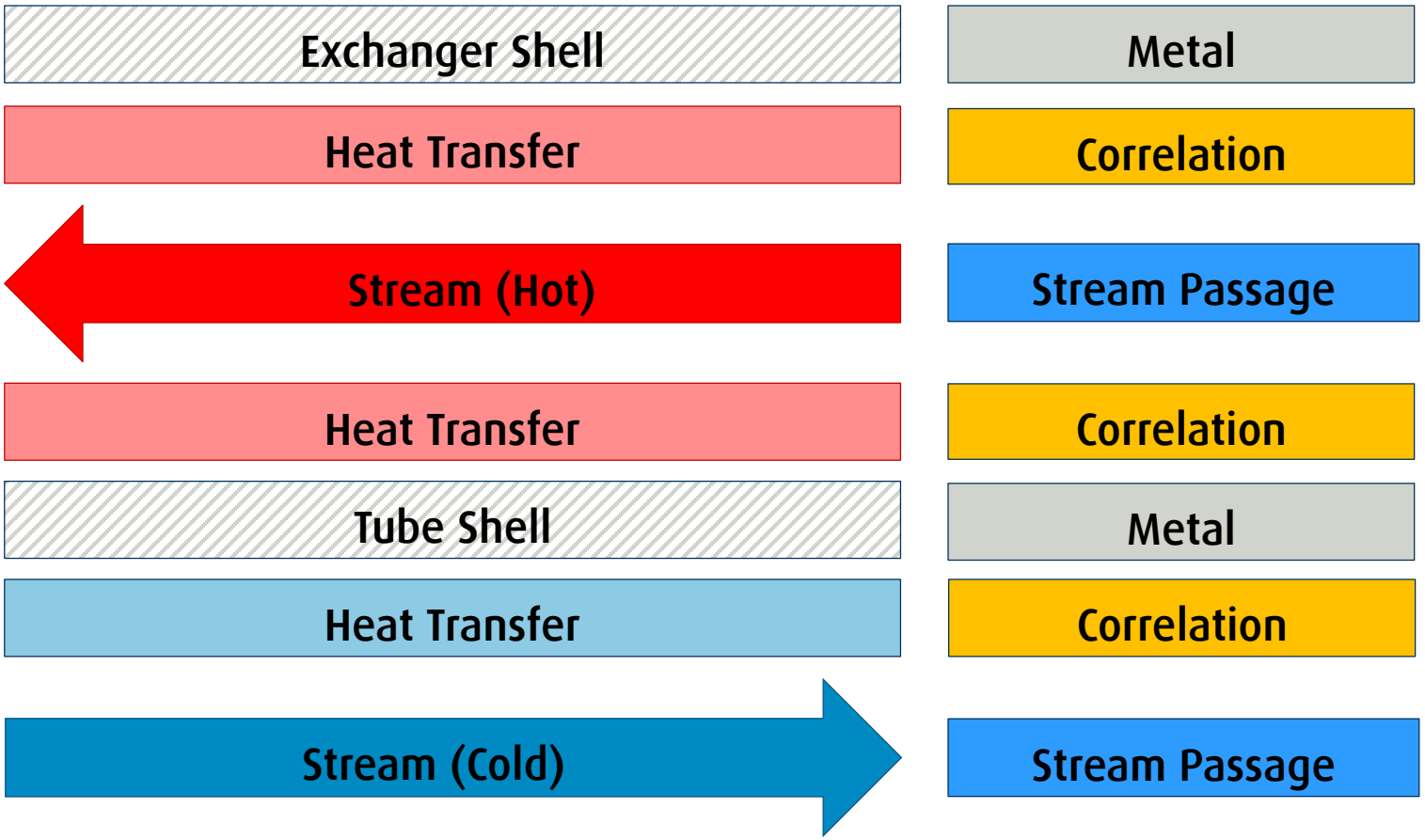
Spiral Wound + Shell & Tube Exchangers – Topology

- Streams inside tube shells
- Streams between tube shells and exchanger shell





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Collaborate. Innovate. Deliver.

Thank you for your attention.

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