Aalto University
School of Science
and Technology

PHYS-E0562 Nuclear Engineering, advanced course
Lecture 9 – System-scale thermal hydraulics

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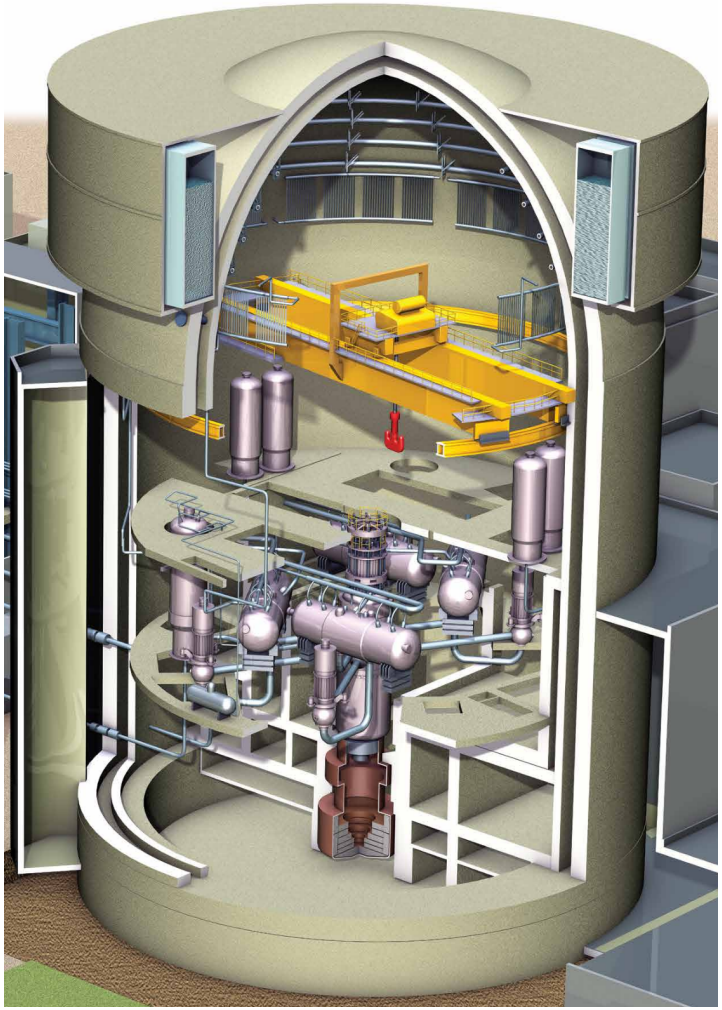
Outline

Introduction to system-scale thermal-hydraulics

System-scale thermal hydraulics

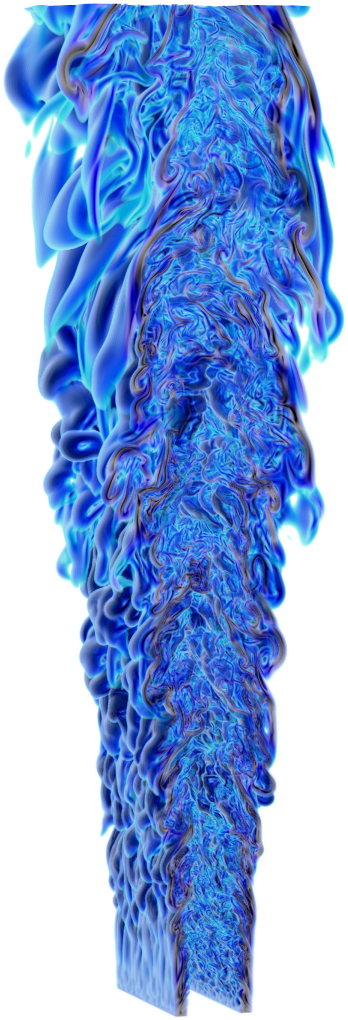


A reactor building and a primary circuit.

Ref: "*AES-2006 (VVER-1200)*" wall chart, Modern Power Systems, 2013.

- In practical safety analyses of nuclear power plants (NPP), it is often necessary to be able to model the power plant coolant system as a whole
- Due to the complexity and the size of power plants, compared to the capabilities of computers today (CPU & memory), rather crude simplifications have to be made to the description of the physical phenomena used as the basis of the simulation code
- Simulation tools based on this kind of highly simplified methods and approaches are called *system-scale codes*, or simply *system codes*
  - Although the methods are in principle simple, the codes are actually very complex due to the very wide parameter ranges and flow regimes they have to cover
- Well-known international system codes include ATHLET, CATHARE, RELAP5, SPACE, TRAC and TRACE. Also worth mentioning is the Finnish system code Apros.

Background: simulation of single-phase flows is complicated



- The behaviour of viscous fluids (e.g. water) seems to be well predicted by the seemingly simple differential equations known as the *Navier-Stokes equations*:

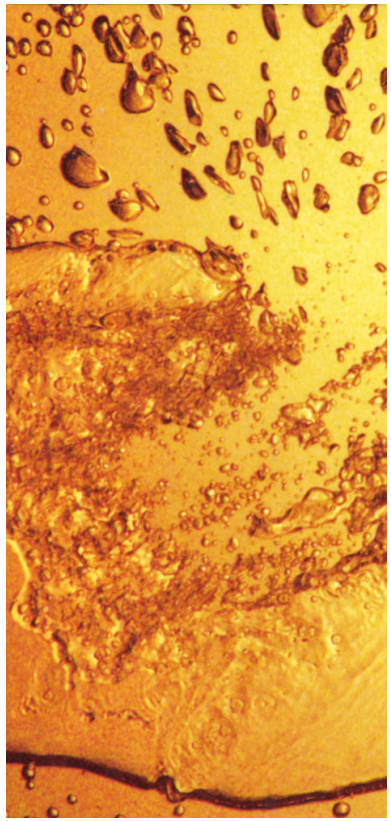
$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} = -\frac{1}{\rho}\nabla p + \mathbf{F} + \nu \nabla^2 \mathbf{u}$$

  - Analytical solutions for the NS-equations can be obtained only in very simple situations
- Numerical solution of fluid flows based *directly* on the NS-equations poses a tremendous challenge for computers (Direct Numerical Simulation, DNS)
  - To directly solve all scales of turbulence, an extremely fine calculation grid has to be used
  - DNS simulation can be performed with modern supercomputers only for very limited calculation domains, and for very short periods of time
- (it is also still unclear whether the NS-equations have a smooth solution in all situations [the existence and smoothness problems]. . .)

Ref: http://exactcodesign.org/sample-page/direct-numerical-simulation

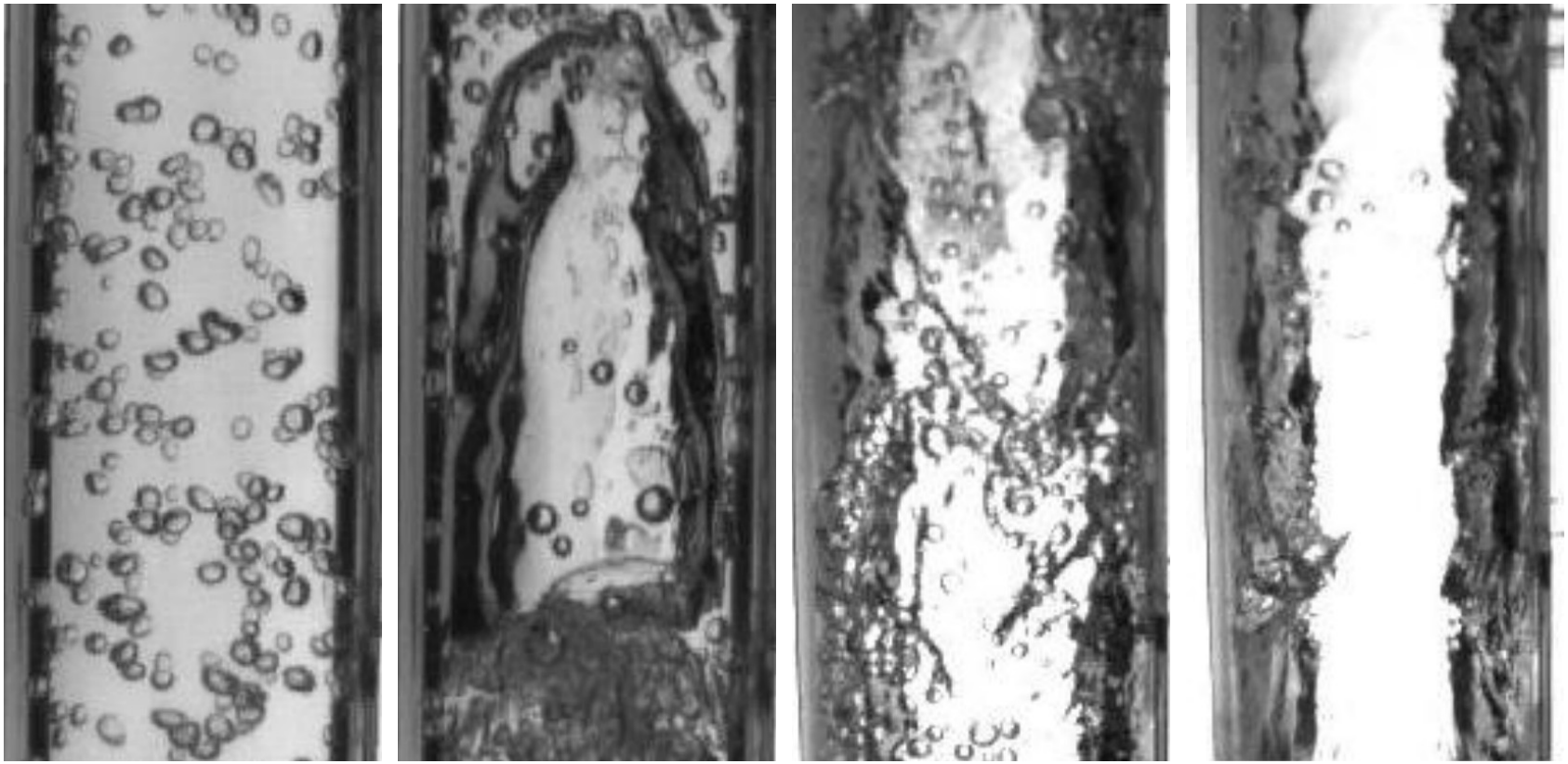
Two-phase flows make things even more complicated

- The NS-equations are applicable only inside continuous regions, i.e. not over the interface between two phases
- The fluid behaviour has to be solved separately in the volumes occupied by each phase, and also the behaviour of the interface has to be solved based on phase movements
- These depend directly on each other, forming a very tightly coupled system:
  - To solve the fluid phase behaviour, the location of the interfaces must be known, as these form the boundaries of the calculation domain
  - To solve the interface behaviour, the behaviour of fluid phases must be known
- Interface tracking or capturing methods can be used in this kind of calculations



Ref: Ishii, M. and Hibiki, T.: "*Thermo-Fluid Dynamics of Two-Phase Flow*", Springer, 2006

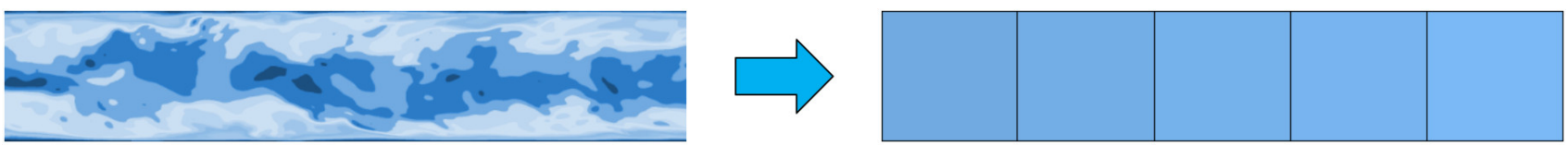
Two-phase flows in practice — Flow regimes in vertical upward flow



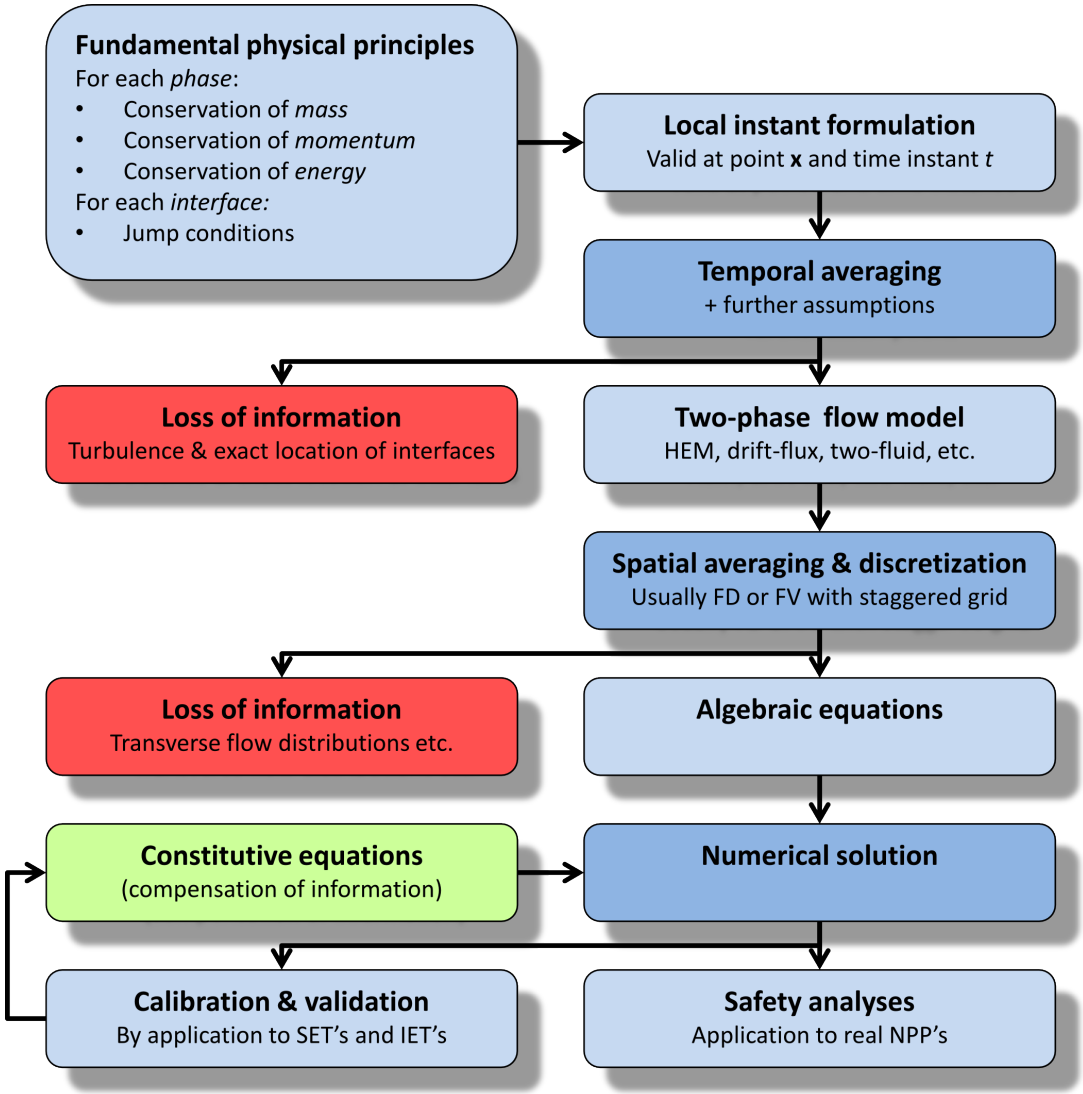
Ref: M. Yadev: "*Geometrical effects of flow restrictions and configurations on interfacial structures in two-phase flow*", M.Sc. Thesis, The Pennsylvania State University, 2009.

Simplifications of the flow equations

- Turbulence models
  - Large eddy simulation (LES): only the larger turbulence scales are solved directly from NS-equations, a model is used for the smaller scales
  - Reynolds-averaged Navier-Stokes (RANS): the NS-equations are decomposed into average and fluctuating parts by time-averaging. The average part is solved directly and a turbulence model is used for the fluctuating part
- The system-scale: further simplifications
  - In system scale the field equations are averaged both in time and in space. Turbulence is largely neglected. Interfacial and wall phenomena have to be modeled.
  - Since flow systems such as the primary circuit of an NPP are mainly built of pipes, one-dimensional flow equations are usually sufficient
- **All simplifications have to be compensated by supplying additional models for specific phenomena**



The approach to system-scale modeling



Flow models and field equations

The local instant formulation

Derivation of the field equations used in a system-code start from the fundamental physical principles of conservation of mass, momentum and energy.

- If a two-phase flow is considered as a field that is divided into single-phasic subregions with moving and deforming boundaries in between, the basic continuum conservation equations (i.e. Navier-Stokes equations) will be valid inside each such subregion
- Appropriate jump conditions need to be imposed on interfaces, and boundary conditions on other boundaries
- The resulting group of equations is called the *local instant formulation*.

$$\frac{\partial \rho_k}{\partial t} + \nabla \cdot (\rho_k \mathbf{u}_k) = 0$$

$$\frac{\partial \rho_k \mathbf{u}_k}{\partial t} + \nabla \cdot (\rho_k \mathbf{u}_k \mathbf{u}_k) = -\nabla p_k + \nabla \cdot \mathbb{T}_k + \rho_k \mathbf{g}_k$$

$$\frac{\partial \rho_k e_k^*}{\partial t} + \nabla \cdot (\rho_k e_k^* \mathbf{u}_k) = -\nabla \mathbf{q}_k + \nabla \cdot (\mathbb{S}_k \cdot \mathbf{u}_k) + \rho_k \mathbf{g}_k \cdot \mathbf{u}_k + \dot{q}_k$$

- These equations are expressed in terms of local (at $\mathbf{x}$) instant (at t) variables, and are indeed valid only inside continuous material regions and not across the interfaces

Averaging operators (1/2)

In order to arrive to practical set of field equations, the local instant equations have to be averaged both in time and in space. In the following, we make the simplifying assumption that the interfaces are infinitesimally narrow, and thus occupy no space.

- First, a phase density function X_k is defined such that

$$X_k(\mathbf{x}, t) \overset{\text{def}}{=} \begin{cases} 1, & \text{point } (\mathbf{x}, t) \text{ is occupied by the phase } k \\ 0, & \text{otherwise} \end{cases},$$

- The Eulerian time average is defined as

$$\overline{F_k}(\mathbf{x}_0, t_0) \overset{\text{def}}{=} \frac{1}{\Delta t} \int_{\Delta t} F_k(\mathbf{x}_0, t)\, \mathrm{d}t.$$

- The phase time average, that is the natural mean value associated with phase k is then defined as

$$\overline{\overline{F_k}} \overset{\text{def}}{=} \frac{\overline{X_k F_k}}{\overline{X_k}}.$$

Averaging operators (2/2)

- For extensive variables, such as momentum and enthalpy, we defined the density-weighted phase time average

$$\widehat{\psi_k} \overset{\text{def}}{=} \frac{\overline{\rho_k \psi_k}}{\overline{\rho_k}} = \frac{\overline{\overline{\rho_k \psi_k}}}{\overline{\overline{\rho_k}}}.$$

- System codes work mainly with one-dimensional description of the flow equations. Thus we define
  - Area-average over the cross-sectional area S is defined as

$$\left\langle F_k \right\rangle \overset{\text{def}}{=} \frac{1}{S} \int_S F_k \, \mathrm{d}S,$$

  - The volume-fraction-weighted area-average as

$$\left\langle\!\left\langle F_k \right\rangle\!\right\rangle \overset{\text{def}}{=} \frac{\left\langle \alpha_k F_k \right\rangle}{\left\langle \alpha_k \right\rangle}.$$

- The temporal averaging has the effect that exact locations of the interfaces are smeared out: from here on the phases are treated as *interpenetrating continua*
- With the area-averaging, all information on the transverse flow distributions will be lost

Flow models and field equations (1/2)

- The macroscopic two-phase flow models arise from applying appropriate averaging operations to the local instant equations. The averaging operators are not necessarily the ones just defined (e.g. statistical average can be used as well).
- The equations arising from the averaging are called the *field equations*: they describe the time-behaviour of each field considered in the model
- Because of the spatial and temporal averaging, additional models are needed to compensate the loss of information. Models are needed for
  - Wall friction ($f_{\mathrm{w},k}$) & heat transfer ($h_{\mathrm{w},k}$) for each field k
  - Interfacial friction ($f_{\mathrm{i},kk'}$) & heat transfer between the field k and each other field k' ($h_{\mathrm{i},kk'}$) (naturally from Newton's third law, $f_{\mathrm{i},kk'} = -f_{\mathrm{i},k'k}$)
- The additional models are called the *constitutive* or the *closure equations*
  - These are typically correlations based on experimental data from separate effect test facilities

Flow models and field equations (2/2)

- Further simplifications can be used to reduce the number of solved field equations in system-scale analyses. Different simplifications result in different flow models:
  - Homogeneous equilibrium model (HEM) (3 equations)
  - Drift-flux model (5 equations)
  - The two-fluid model (6 equations)
  - Multi-field models ($3n$ equations)
- The main difference between the flow models is in how many field equations are used to describe the fluid flow
- In theory, more field equations means less assumptions, and thus should result in more accurate predictions
  - On the other hand, more field equations also means that more constitutive equations are needed, so the results become more and more affected by the quality of the constitutive models
  - In addition, the quantities that have to be estimated for formulating the constitutive models become more more difficult to measure with refinement of the flow model

The homogeneous equilibrium model

- The homogeneous equilibrium model is the simplest two-phase flow model. The assumptions are
  - The two-phase fluid forms a homogeneous mixture $\rightarrow u_{\mathsf{l}} = u_{\mathsf{g}}$
  - The fluid phases are in thermal equilibrium $\rightarrow$ when both phases present $T_{\mathsf{l}} = T_{\mathsf{g}} = T_{\mathsf{sat}}$
- The field equations are written only for the mixture (3 equations). The time-averaged HEM model field equations in three-dimensional form with some simplifications are

$$\frac{\partial \overline{\rho}}{\partial t} + \nabla \cdot (\overline{\rho}\widehat{\mathbf{u}}) = 0$$

$$\frac{\partial \overline{\rho}\widehat{\mathbf{u}}}{\partial t} + \nabla \cdot (\overline{\rho}\widehat{\mathbf{u}}\widehat{\mathbf{u}}) = -\nabla \overline{p} + \overline{\rho}\widehat{\mathbf{g}} + \mathbf{F}_{\mathsf{w}}$$

$$\frac{\partial \overline{\rho}\widehat{h}}{\partial t} + \nabla \cdot (\overline{\rho}\widehat{h}\widehat{\mathbf{u}}) = \frac{\partial \overline{p}}{\partial t} + q_{\mathsf{w}} + \overline{\rho}\widehat{\mathbf{u}}\widehat{\mathbf{g}}$$

- Constitutive modelling is needed for
  - Wall friction of the mixture (one equation): $\mathbf{F}_{\mathsf{w}}$
  - Wall heat transfer to the mixture (one equation): q_{w}
  - (The HEM assumption corresponds to $f_{\mathsf{i}}, h_{\mathsf{ig}}, h_{\mathsf{il}} = \infty$)
- The HEM model can be used in simplest two-phase scenarios, but the assumption of equal velocities restricts its use from such important situations as reflooding of nuclear reactor core

Drift-flux models

- In drift-flux models, only the momentum of the mixture as a whole is conserved, and the velocity difference between the phases is accounted for with a (drift-flux) correlation
  - The continuity equations are written separately for each phase
  - The momentum equation is written only for the mixture
    - The velocities are deduced from the drift velocity based on the used correlation
  - The thermal equilibrium equations are written either for the mixture (4-eq. model), or separately for each phase (5-eq model)
- Constitutive modeling is needed for
  - Wall heat transfer to the mixture of to both the phases (one/two equations)
  - Wall friction for the mixture (one equations)
  - Interfacial heat transfer coefficients (zero/two equations)
  - Drift velocity (one equation, the drift-flux model defines $f_{\mathrm{i},kk'}$ implicitly)
- The use of drift-flux model is limited to states in which the used drift-flux correlation is valid
- Drift-flux models are not able to accurately predict situations in which inertial forces have a strong effect on the relative velocity between phases

The two-fluid model

In the two-fluid model, no further assumptions are made; both the liquid and gas phase are considered independently of each other

- The continuity-, momentum-, and the energy equations are written separately for each phase
- Constitutive modelling is needed for
  - Wall heat transfer to both the phases (two equations)
  - Wall friction of both the phases (two equations)
  - Interfacial heat transfer coefficients (two equations)
  - Interfacial friction coefficient (one equation)
- The two-fluid model is in theory more accurate than drift-flux models, but as the interfacial friction coefficients in the two-fluid models is often modelled using drift-flux correlations there are no big differences in many situations
- In the next slide, the one-dimensional two-fluid model field equations are presented. Field equations for the simpler models are very similar to these with the obvious simplifications.

The one-dimensional two-fluid model

The continuity equation for phase k

$$\frac{\partial}{\partial t} S\langle \alpha_k \rangle \overline{\overline{\rho_k}} \langle\langle \widehat{u_{z,k}} \rangle\rangle + \frac{\partial}{\partial z} S\langle \alpha_k \rangle \overline{\overline{\rho_k}} \langle\langle \widehat{u_{z,k}} \rangle\rangle = S\langle \Gamma_k \rangle$$

The momentum equation for phase k

$$\begin{aligned}
&\frac{\partial}{\partial t} S\langle \alpha_k \rangle \overline{\overline{\rho_k}} \langle\langle \widehat{u_k} \rangle\rangle + \frac{\partial}{\partial z} S\langle \alpha_k \rangle \overline{\overline{\rho_k}} C_{uk} \langle\langle \widehat{u_{z,k}} \rangle\rangle^2 = -S\langle \alpha_k \rangle \frac{\partial}{\partial z} \langle\langle \overline{\overline{p_k}} \rangle\rangle \\
&\quad + \frac{\partial}{\partial z} S\langle \alpha_k \rangle \langle\langle \overline{\overline{\tau_{k,zz}}} + \tau^{\mathsf{T}}_{k,zz} \rangle\rangle - U \alpha_{\mathsf{w}k} \tau_{\mathsf{w}k} + \langle \alpha_k \rangle \overline{\overline{\rho_k}} \widehat{g_z} \\
&\quad + S\langle \Gamma_k \rangle \langle u_{\mathsf{i}k} \rangle + \left(\langle\langle \overline{\overline{p_{\mathsf{i}k}}} \rangle\rangle - \langle\langle \overline{\overline{p_k}} \rangle\rangle \right) \frac{\partial}{\partial z} S\alpha_k + S\langle \mathbf{M}_{\mathsf{i}k} - \nabla \alpha_k \cdot \overline{\overline{\tau_{\mathsf{i}k}}} \rangle_z
\end{aligned}$$

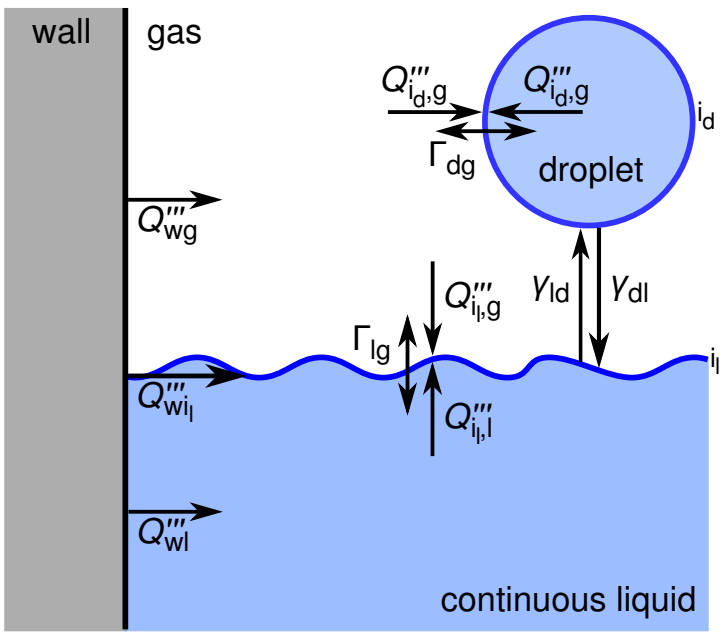
The total energy equation for phase k

$$\begin{aligned}
&\frac{\partial}{\partial t} S\langle \alpha_k \rangle \overline{\overline{\rho_k}} \langle\langle \widehat{h^*_k} \rangle\rangle + \frac{\partial}{\partial z} S\langle \alpha_k \rangle \overline{\overline{\rho_k}} C_{hk} \langle\langle \widehat{h^*_k} \rangle\rangle \langle\langle \widehat{u_k} \rangle\rangle = -\frac{\partial}{\partial z} S\langle \alpha_k \rangle \langle\langle \overline{\overline{q_k}} + q^{\mathsf{T}}_k \rangle\rangle_z \\
&+ U \alpha_{\mathsf{w}k} q''_{\mathsf{w}k} + \frac{\partial}{\partial z} S\langle \alpha_k \rangle \langle\langle \overline{\overline{\tau_{k,zz}}} \widehat{u_{z,k}} \rangle\rangle + S\langle \alpha_k \rangle \overline{\overline{\rho_k}} \widehat{g_z} \langle\langle \widehat{u_{z,k}} \rangle\rangle + S\langle \Gamma_k \rangle \langle \widehat{h^*_{\mathsf{i}k}} \rangle + S\langle a_{\mathsf{i}} \overline{\overline{q''_{\mathsf{i}k}}} \rangle \\
&\quad + S\langle \left(\overline{\overline{p_k}} - \overline{\overline{p_{\mathsf{i}k}}} \right) \frac{\partial \alpha_k}{\partial t} \rangle + S\langle \alpha_k \frac{\partial \overline{\overline{p_k}}}{\partial t} \rangle + S\langle \left(\mathbf{M}_{\mathsf{i}k} - \nabla \alpha_k \cdot \overline{\overline{\mathbb{T}_{\mathsf{i}k}}} \right) \cdot \widehat{\mathbf{u}_{\mathsf{i}k}} \rangle_z + S\langle W^{\mathsf{T}}_{\mathsf{i}k} \rangle
\end{aligned}$$

Multi-field models

Multi-field models consider more than two fields separately, to allow more accurate predictions under some special circumstances Additional fields can be introduced by considering that one phase may be composed from separate parts that are somehow distinct from each other

- Liquid: continuous liquid + droplets of different sizes and shapes
- Gas: continuous gas + bubbles of different sizes and shapes



- The most prominent multi-field model is the three-field model with dispersed droplets as the additional field
  - The continuity-, momentum-, and the energy equations are written separately for each phase
- Constitutive modelling is needed for
  - Wall heat transfer for each (n equations)
  - Wall friction for each phase (n equations)
  - Interfacial heat transfer coefficients (two equations for each interface)
  - Interfacial friction coefficient (one equation for each interface)
- In practice, the use of multi-field models is limited by the quality of the constitutive models

Constitutive modeling

Constitutive modeling

- Constitutive models are needed for compensating the loss of information that resulted from averaging the field equations
- They provide equations for source terms in the macroscopic field equations, and in this sense close the system of equations. This is why they are also called *closure laws*
- Typically the closure laws are empirical correlations based on measurements in simplified geometries and situations
  - The correlations are always based on steady-state measurements, but need to be utilized in transient conditions also
  - Often the parameter ranges used in deriving the correlations are seriously limited, but the correlations still need to be used in the general case
  - Usually the correlations are tuned during the validation process of a code, so that best possible prediction is obtained

Need for closure laws

- The number of needed constitutive equations depends on the flow model:

HEM model: 2 closure laws	Drift-flux model (5-eq.): 6 closure laws	Two-fluid model (6-eq.): 7 closure laws
1 x wall heat transfer 1 x wall friction	2 x wall heat transfer 1 x wall friction 2 x interfacial heat transfer 1 x drift flux	2 x wall heat transfer 2 x wall friction 2 x interfacial heat transfer 1 x interfacial friction

- In theory, the flow models become more accurate with the addition of new field equations (3-equation $\rightarrow$ 5-equation $\rightarrow$ 6-equation)
  - In practice this is not necessarily so, because of difficulties with formulating accurate closure laws
  - Especially the closure laws dealing with interfacial phenomena are difficult to produce
- In the following slides, examples of different closure laws that have been utilized in the system code Apros are presented. The presented equations are just a small subset of all constitutive equations included in the code, but should serve as an overview on what kind of equations are used in practice.

Wall friction (1/2)

- The wall friction term is written as

$$F_{\mathrm{w}k} = -\frac{1}{2}\frac{f_k \rho_k u_k |u_k|}{D_{\mathrm{h}}}$$

- The friction factor f_k is calculated by multiplying a single-phase friction factor with a two-phase multiplier c_k:

$$f_k = f_{\text{single-phase},k} \cdot c_k$$

- The single-phase friction factor is calculated separately for laminar flow ($\mathrm{Re} < 4000$) and turbulent flow ($\mathrm{Re} > 2300$) and the final value is interpolated from these
- The equations used for laminar and turbulent single-phase flows could be for example

$$f_{\text{laminar},k} = \frac{64}{\mathrm{Re}_k}, \qquad f_{\text{turbulent},k} = \frac{1}{(1.82 \cdot \log_{10}(\mathrm{Re}_k) - 1.64)^2}$$

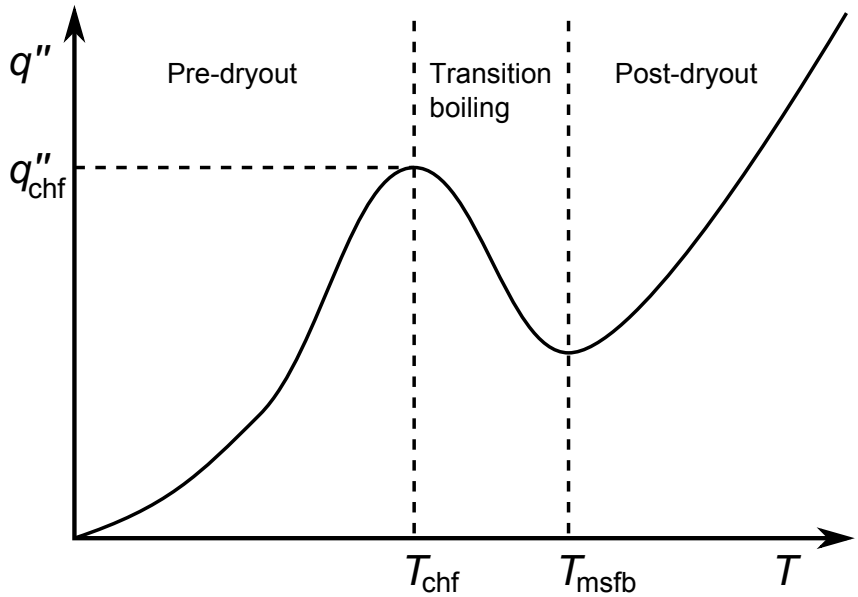
Wall friction (2/2)

- The two-phase friction multiplier tries to take into account the distribution of phases in a flow channel ($\sim$ what part of the channel wall is in contact with each phase)
  - Is the flow annular (only liquid touches the wall) or inversed-annular (only gas is in wall contact)?
  - Is the flow stratified (horizontal pipes)?
- The code has to try to deduce these based on the local variables: void fraction, fluid and wall temperatures, flow velocities, etc.
- Also in transition from laminar to turbulent, we interpolate between different equations mainly to make the closure law continuous. There is no physical justification for this choice
  - In fact, we know that the turn to turbulence happens stochastically at some point in the Reynolds interval of 2300 to 4000...

Wall heat transfer (1/2)

Wall heat transfer is more complicated to model than wall friction. Models are needed for:

- Pre-dryout natural convection (laminar & turbulent)
- Pre-dryout forced convection (l & t)
- Nucleate boiling
- Transition boiling
- Film boiling
- Post-dryout natural convection (l & t)
- Post-dryout forced convection (l & t)
- Radiation heat transfer from wall to fluid



Also the heat transfer region and flow regime has to be deduced before appropriate correlation can be selected. For this reason estimates are needed for

- The critical heat flux (CHF)
- Minimum stable film boiling temperature, T_{msfb} ($\sim$ Leidenfrost temperature)

Wall heat transfer (2/2)

- Correlations for wall heat transfer are usually formulated in terms of the dimensionless Nusselt number: $\mathrm{Nu} \overset{\text{def}}{=} hD/\lambda$
- Forced convection (both in pre- and post-dryout conditions) can be predicted to a reasonable accuracy by the Dittus-Boelter correlation originally developed for automobile radiators in 1930:

$$\mathrm{Nu}_{\mathrm{fc},k} = 0.023 \cdot \mathrm{Re}_k^{0.8} \mathrm{Pr}_k^{0.4}$$

- Nucleate boiling heat transfer can be predicted with the Thom correlation

$$\mathrm{Nu}_{\mathrm{nb}} = 1971.2 e^{2p/8687000} (T_{\mathrm{w}} - T_{\mathrm{sat}}) \frac{\lambda_{\mathrm{l}}}{D}$$

- Transition boiling is somewhat similar to the laminar-turbulent transition with wall friction in that the change from film boiling back to nucleate boiling (i.e. rewetting) occurs stochastically at some point when the heat flux is decreased. The solution to this problem is also similar: transition boiling can be modelled with interpolating between the critical heat flux and the heat flux corresponding to the minimum stable film boiling temperature.

Critical heat flux

- For critical heat flux, there exists a large number of correlations. Unfortunately this phenomenon is heavily dependent on the geometry, so typically nuclear fuel manufacturers make measurements and provide a specific correlation for their specific fuel bundle type
- In a general-purpose code, such specific correlations cannot be used, but instead something more general is preferred
- Typically this means CHF correlations obtained with pipe measurements. Examples of these are the Biasi correlation and the CHF look-up tables of Groeneveld et al.

	X→	-0.50	-0.40	-0.30	-0.20	-0.15	-0.10	-0.05	0.00	0.05	0.10	0.15	0.20	0.25	0.30	0.35	0.40	0.45	0.50	0.60	0.70	0.80	0.90	1
12000	0	4070	3883	3698	3525	3433	3322	3163	2914	2391	1936	1606	1334	1173	1026	909	814	745	694	588	397	225	141	0
12000	50	4436	4247	4061	3869	3770	3658	3506	3285	2784	2367	2081	1857	1694	1565	1498	1357	1200	1087	867	667	381	242	0
12000	100	5023	4806	4538	4290	4171	3983	3844	3645	3267	2878	2711	2500	2257	2069	1905	1622	1460	1290	977	772	446	301	0
12000	300	5366	5081	4741	4434	4269	4138	3950	3838	3516	3199	2912	2701	2467	2285	2108	1940	1830	1630	1250	840	500	316	0
12000	500	5647	5188	4869	4445	4298	4131	3988	3819	3555	3240	2951	2724	2500	2310	2160	1875	1678	1474	1011	423	296	205	0
12000	750	6233	5596	5072	4528	4310	4067	3904	3659	3418	3067	2773	2526	2277	2039	1798	1396	1180	989	312	251	211	131	0
12000	1000	7031	6267	5500	4700	4430	4100	3855	3447	3243	2878	2516	2291	1905	1640	1420	1073	920	310	214	118	78	76	0
12000	1500	8214	7105	6221	5242	4662	4271	3813	3405	2952	2526	2112	1723	1389	1096	918	377	315	205	105	41	39	36	0
12000	2000	8959	7711	6598	5472	4982	4417	3841	3375	2830	2300	1816	1410	1109	911	385	119	110	77	71	50	37	31	0
12000	2500	9851	8471	7225	5977	5407	4720	3900	3367	2739	2119	1603	1215	971	753	293	172	139	119	99	59	40	27	0
12000	3000	10436	9128	7655	6409	5706	4923	3949	3364	2690	1985	1492	1101	889	689	354	300	245	195	154	81	45	26	0

Ref: Groeneveld, D. C. et al.: "*The 2006 CHF look-up table*", Nuclear Engineering and Design, Vol. 237, No. 15, 2007

Numerical solution methods

Difficulty of solving the field equations

- The six independent variables in the two-fluid model are
  - Pressure p
  - Phase velocities u_{l} and u_{g}
  - Enthalpies h_{l} and h_{g} (or internal energies e_{l} and e_{g}, or temperatures T_{l} and T_{g})
  - Void fraction α
- These have to be solved from the (six) field equations. If pressures are known (or treated explicitly), the new velocities can be solved from the momentum equations. Likewise, if the velocities and pressures are known void fractions and enthalpies are easy to solve from the continuity and energy equations.
- The problem, however, is that
  a) The field equations form a particularly tightly coupled system: the continuity and momentum equations link pressures and velocities together in a way that one cannot be assumed constant while the other is changing
  b) The pressure only appears through the gradient term in the momentum equations (+ possibly as a source term in the thermal energy equations)
- In practice these mean that the variables cannot be solved in a sequential one-by-one fashion

A few words on discretization

For numerical solution, the field equations have to be discretized both in time and in space

- The temporal discretization is inherently connected to the used solution method (implicit or semi-implicit). Fully-implicit solutions are more demanding to obtain, but are otherwise more desirable

$$y^{n+1} - y^n = f(y^{n+1}, t + \Delta t) \qquad \text{vs} \qquad y^{n+1} - y^n = \Delta t f(y^n, t)$$

- First-order upwind scheme is most often used in spatial discretization for the convection terms

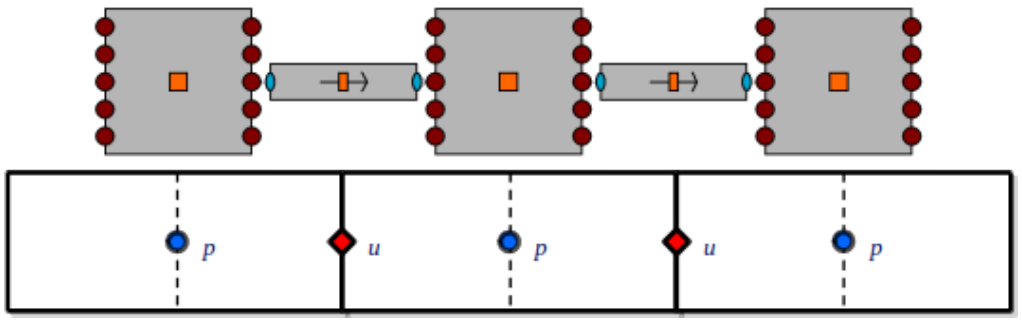
$$\left(\frac{\partial u}{\partial z}\right)_i \approx \begin{cases} (u_i - u_{i-1})/\Delta z, & \text{if } u_i \geq 0 \\ (u_{i+1} - u_i)/\Delta z, & \text{otherwise} \end{cases}$$

  - This results in a stable and robust solution scheme, but is also associated with high level of numerical diffusion
- The actual spatial discretization (i.e. at which point in the system under study the solution is required) is done by the user of the system code when building the simulation model
  - In system-scale analyses, the calculation domain (e.g. a primary circuit of an NPP) is divided into calculation cells with lengths typically between 10 cm and a few meters

The staggered grid discretization scheme

Practically all the system-scale codes utilize the so-called staggered grid discretization

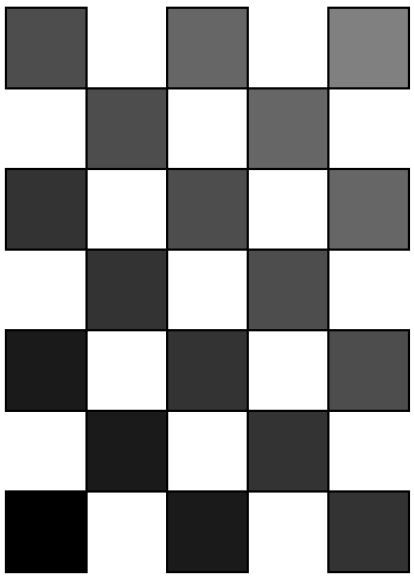
- In the staggered discretization scheme, the momentum equations are discretized at different points than the other (scalar) field equations
  - Pressures, enthalpies and void fractions are solved in the centre of a calculation cell
  - Velocities are solved at the boundaries of cells
- The calculation cells of the pressure grid are called *(scalar) nodes*, and the calculation cells of the momentum grid are called *junctions*, *branches* or *vector nodes*



Elimination of the checker board phenomenon

The staggered grid discretization enhances the stability of the numerical solution scheme and eliminates the well-known checker-boarding problem associated with the collocated grid scheme

- The checker boarding phenomenon originates from typical discretizations in collocated grid arrangement, and is a result of the velocity and pressure field becoming locally decoupled



- According to the momentum equations, velocity u at cell i is proportional to the pressure gradient

$$u_i \sim (\nabla p)_i$$

- Pressure gradient at cell i is discretized as

$$(\nabla p)_i = \frac{p_{i+1/2} - p_{i-1/2}}{\Delta z} \rightarrow \frac{p_{i+1} - p_{i-1}}{2\Delta z}$$

- Thus u_i is not directly related to p_i, making solutions exhibiting a checker-board kind of behavior valid from the numerical point of view

The fully-implicit method (1/2)

Solving all the field equations with fully-implicit discretization (all terms discretized at $t + \Delta t$) at the same time is possible with the general approach used with non-linear PDE's: generalized Newton's method

- Such solution method is used in the codes CATHARE, ATHLET and RELAP-7
- The drawback with this approach is that the matrix that has to be inverted (the Jacobian of the coefficient matrix) becomes relatively large ($\sim 6N \times 6N$, where N is the number of calculation cells), and consequently the inversion is time consuming, especially in three-dimensional situations in which the coefficient matrix is much more dense than in 1D situations
- Also, the Jacobian has to be formed analytically, which in practice means writing a lot of differentials into the code. However, this can be circumvented through

  a) numerical estimation of the Jacobian (consumes twice as much time as evaluating directly from analytic expression)

  b) using a Jacobian-free Newton-Krylov method (JFNK), in which only the approximate effect (via matrix-vector product) of the Jacobian has to be calculated

The fully-implicit method (2/2)

The fully-implicit solution based on the generalized Newton's method proceeds as follows

- All solved variables (p, u_l, u_g, h_l, h_g, α) for all calculation cells are stored in a vector $\mathbf{x}$, and the field equations are discretized as

$$\mathbf{F}(\mathbf{x}) = 0$$

- The solution is then found by repeatedly solving $\mathbf{x}^{n+1}$ from

$$\mathbf{J}(\mathbf{x}_{n+1} - \mathbf{x}_n) = -\mathbf{F}(\mathbf{x}_n), \qquad \mathbf{J} \overset{\text{def}}{=} \partial\mathbf{F}/\partial\mathbf{x}$$

- The iteration is continued until convergence: $-\mathbf{F}(\mathbf{x}_n) \approx 0$
- The fully-implicit solution method is unconditionally stable, which means that the stability of the solution doesn't pose limitations to the used time step

Numerical solution schemes

The other option is to use the operator-splitting approach with a semi-implicit discretization (part of the terms discretized at $t + \Delta t$ and rest at t):

- The new velocities are solved from the momentum equations as function of new pressures:
$$u_{k,i+1/2}^{n+1} = v_{k,i+1/2} + D_{k,i+1/2}(p_{i+1}^{n+1} - p_i^{n+1})$$
- These expressions are then used to eliminate the velocities in either just the continuity equations, or in continuity and energy equations, to form a linear equations group in which the only unknowns are the new pressures p_i^{n+1}
- With the pressures solved, the new velocities are obtained from the above momentum expressions, and finally the scalar values can be solved using the new velocities
- The non-iterative semi-implicit methods result in very fast calculation speed (low computational cost of a single time step), but on the other hand, the time steps sizes are limited by the material CFL condition ($u\Delta t/\Delta z < 1$)
  - This condition may be relaxed through the use of predictor-corrector type fractional step methods (e.g. the “Nearly implicit method” and the “Stability-enhancing two-step method”)
- This kind of methods are used in the computer codes RELAP5, TRAC, TRACE and SPACE

Fully-implicit solution through iteration

- Apros uses a numerical method that is somewhat similar to the SIMPLE method used in CFD codes, or can also be understood as an iterative version of the semi-implicit methods desribed in the previous slide. The method proceeds roughly as follows:
  - Momentum equation is discretized similarly to what was done with semi-implicit methods, and an expression for the new time velocities as function of pressures is obtained

$$u^{n+1} = v + D\nabla p^{n+1}$$

  - This expression is then used to eliminate the velocities in the continuity equations, thus resulting in a linear system of equations containing pressure as the only unknown
  - The pressures are then solved, and the new time velocities are calculated from the expression above
  - The new velocities are then used for solving void fractions and phase enthalpies
  - This loop is iterated until convergence. Key difference to the non-iterative semi-implicit methods is that the current iteration values are used for all explicit terms
- This method is slightly less robust than the fully-implicit method
- Due to treating some of the terms explicitly, the convergence rate is lower (more iterations are in general needed)
- The method also has a few numerical dials of which the user should be aware of, such as the under-relaxation factors

A few words on hyperbolicity (1/2)

- Mathematical models describing physical phenomena should always be well posed, which requires that
  a) A unique solution to the problem exists
  b) The solution depends continuously on the initial and boundary conditions
- In practice the well-posedness of a problem is difficult to show directly, but it is known that hyperbolic partial differential equations form a well-posed initial value problem
- However, the two-fluid model field equations with a single pressure as such are non-hyperbolic, and thus it may not be possible to find a unique continuously-changing solution for them in all situations

A few words on hyperbolicity (2/2)

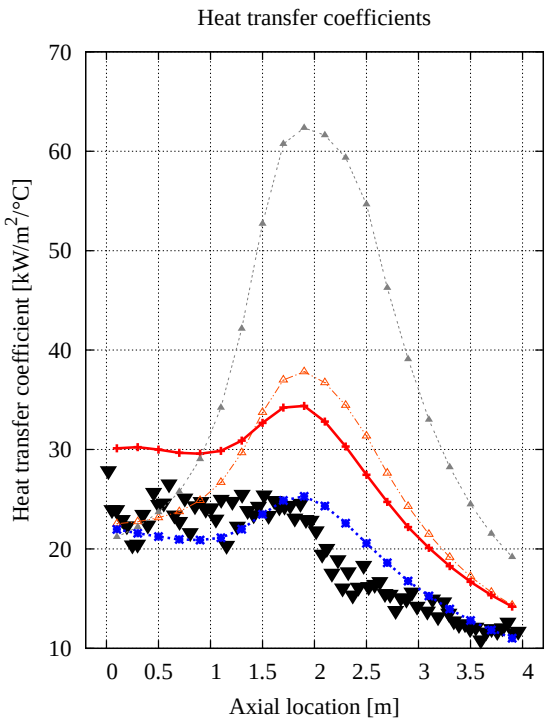
- In practice it has been observed, that the when non-hyperbolic two-fluid model is solved with a system code, a unique solution is usually found if the node sizes are not too small
  - It turns out that the numerical diffusion originating from using first-order upwind discretization renders the equations hyperbolic
  - However, the magnitude of this numerical diffusion is related to node lengths, and approaches zero with $\Delta z \rightarrow 0$. Thus the numerical diffusion can renderer the system of equations hyperbolic only above some limit $\Delta z > (\Delta z)_{\text{min}}$
  - This prohibits mesh convergence studies, i.e. the normal way of assuring that the numerical solution is a solution of the original mathematical model
- In some system codes, such as in CATHARE, and RELAP-7, an effort has been made for making the field equations inherently hyperbolic
  - This happens by formulating the closure laws related to interfacial phenomena (interfacial pressure and virtual mass terms) so that all the characteristic velocities of the system are real, or by allowing different pressures for the phases (a 7-equation two-fluid model)
  - As a consequence very small cell sizes can be used, which is convenient for example in modelling critical flows

Limitations of system-scale modeling

Confidence in the simulation results

At this point it should be evident, that the system-scale codes use very crude and in some cases arguably questionable simplifications to achieve their goal

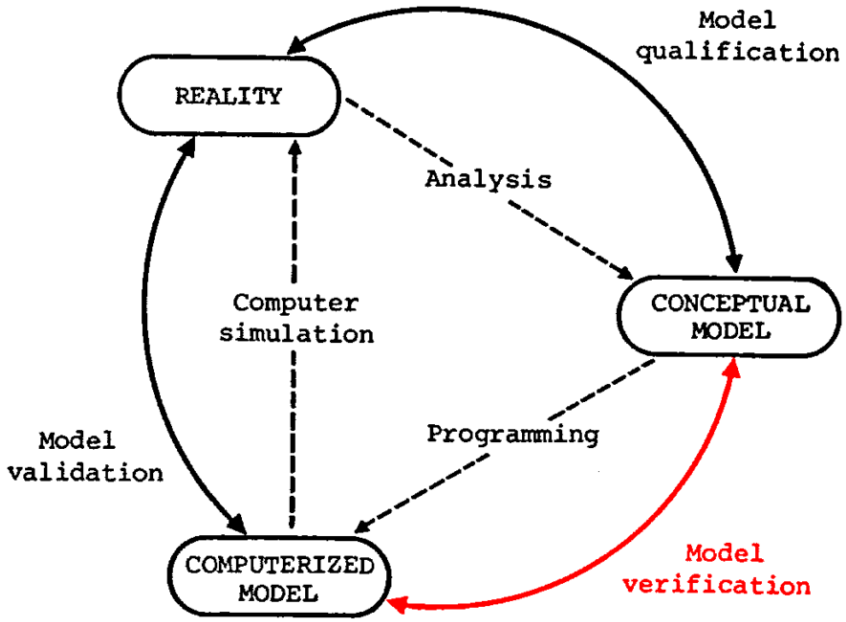
- A question then rises on validity of all the approximations and simplifications used in developing the simulation tool



- **Confidence in the simulation results obtained with system-scale tools is established through an extensive verification and validation effort**
- The approach with system-scale modelling could perhaps be described as deliberately making (more or less) bad assumptions, crude approximations and simplifications, and then in the end *determining how wrong these choices were*
- **Inaccurate results can be acceptable as long as the reasons for the inaccuracies are known and well understood, and the associated uncertainties are quantified**

Verification

Verification process is used to assure that the implementation of a model closely corresponds to the conceptual description provided by the model's developer



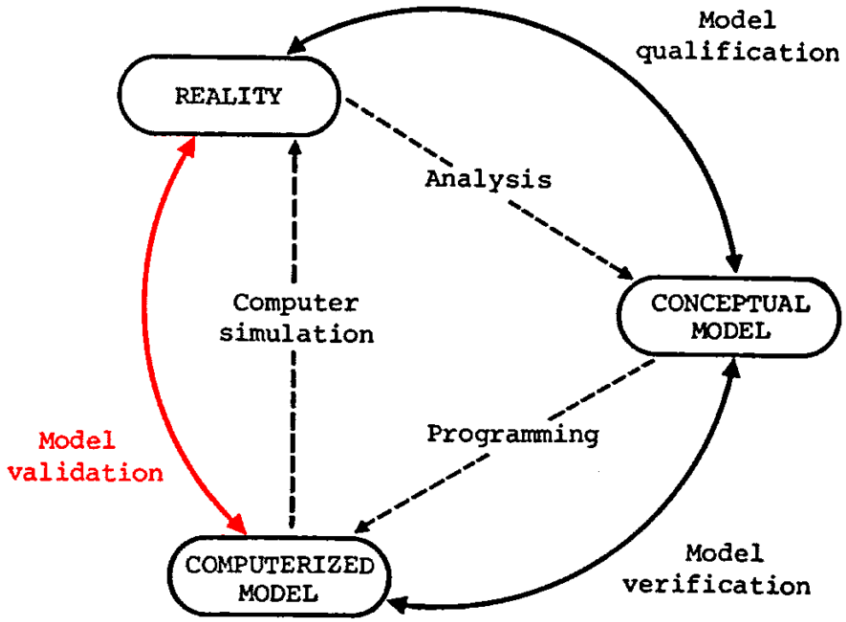
Ref: Schlesinger, S. et al.: "*Terminology for model credibility*", Simulation, Vol. 32, No. 3, 1979

- Computational models have been correctly implemented based on the conceptual models
- The computational models behave like the conceptual models in all situations
- In other words, all errors possibly introduced in implementing the model are weeded out

"Solving the equations right"

Validation

Validation process is used to determine, how closely a computational model corresponds to the physical reality on a certain parameter range



Ref: Schlesinger, S. et al.: "*Terminology for model credibility*", Simulation, Vol. 32, No. 3, 1979

- Computational results are compared to experimental data
- The aim is to determine uncertainties related to the model, but remembering that also the experimental data may be biased and contain random errors
- Validation is applicable only in the parameter ranges covered by experimental data

"Solving the right equations"

Experimental programs and validation matrices

- Extensive thermal-hydraulic experimental programs have been carried out to support the development of system codes.
  - Majority of the experimental work was carried out during the late 1970's and the 1980's in relation to the deployment of the two-fluid model
  - Basically two kinds of experiments are carried out: *separate effect tests* (SET's) and *integral effect tests* (IET's)
    - SET's deal with a single phenomenon at a time. They are used to develop and assess specific correlations in the codes
    - IET's correspond to the real analysis use of the codes; multiple physical phenomena play a role simultaneously. They are used for assessing the overall reliability and accuracy of the code.
- Later the results of these programs have been combined in so-called *validation matrices* developed in an international effort coordinated by OECD/NEA. The validation matrices:
  - Provide a list of known test facilities
  - Describes their capabilities
  - Contain cross-reference tables for suitability for validation of models for different physical phenomena
- Further international cooperation in this field is carried out in the form of the *international standard problems* (ISPs), other OECD/NEA experimental projects and benchmark exercises

Excerpt from a validation matrix

Phenomena		Separate Effects Test Facilities																				
LEGEND x suitable for model validation o limited suitability for model validation - not suitable for model validation							3. France															
		MOBY-DICK	SUPER MOBY-DICK	CANON and SUPER CANON (Horiz)	VERTICAL CANON		TAPIOCA (Vertical)	DADINE (Vertical Tube, Inside)	PERICLES Rectangular	PERICLES Cylindrical	PATRICIA GV 1	PATRICIA GV 2	ERSEC Tube (Inside)	ERSEC Rod Bundle	OMEGA Tube (Inside)	OMEGA Rod Bundle	ECTHOR Loop Seal (Air/Water)	COSI	SUPER MOBY-DICK TEE	PIERO (Air/Water)	EPOPEE	EVA
	Facility No. Info Sheet available	1 a	2 a	3 a	4 a	5	6 a	7 a	8 a	9 a	10 a	11 a	12 a	13 a	14 a	15 a	16 a	17 a	18 a	19 a	20	21 a
0 BASIC PHENOMENA	1 Evaporation due to Depressurisation	x	x	x	x		x	-	-	-	-	-	-	-	o	o	-	-	-	-	-	-
	2 Evaporation due to Heat Input	-	-	-	-		-	o	-	-	-	-	o	o	o	o	-	-	-	-	-	-
	3 Condensation due to Pressurisation	-	-	-	-		-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	4 Condensation due to Heat Removal	-	-	-	-		-	-	-	-	o	-	-	-	-	-	-	o	-	-	-	-
	5 Interfac. Frict. Vertic. Flow	-	-	-	o		o	x	-	-	-	o	-	-	o	o	o	-	-	-	-	-
	6 Interfac. Frict. Horiz. Flow	-	-	o	-		-	-	-	-	-	-	-	-	-	-	o	o	-	-	-	-
	7 Wall to Fluid Friction	x	x	x	-		-	-	-	-	-	-	-	-	-	-	-	-	x	-	-	-
	8 Press. Drops at Geometr. Discontinuities	-	x	-	o		o	-	-	-	-	-	-	-	-	-	-	-	x	-	-	-
	9 Pressure Wave Propagation																					
1 CRITICAL FLOW	1 Breaks	-	x	x	x		x	-	-	-	-	-	-	-	x	x	-	-	x	-	-	-
	2 Valves	-	-	-	-		-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	3 Pipes	x	x	-	-		-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
2 PHASE SEPARATION/VERTICAL FLOW WITH AND WITHOUT MIXTURE LEVEL	1 Pipes/Plena	-	-	-	x		x	o	-	-	o	x	-	-	-	-	-	-	-	o	-	-
	2 Core	-	-	-	-		-	-	x	x	-	-	-	-	-	-	-	-	-	-	-	-
	3 Downcomer	-	-	-	-		-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-

Ref: OECD/NEA: "*Separate Effects Test Matrix for Thermal-hydraulic Code Validation, Volume I: Phenomena Characterisation and Selection of Facilities and Tests*", 1993

Dealing with uncertainties

- As a result of the validation work, an understanding of the accuracy and reliability of the simulation results obtained with a code should be obtained
- When performing safety analyses, in which one must show that the safety margins (e.g. peak cladding temperature (PCT), maximum centre-line temperature (MCT) < T_{limit}), these uncertainties have to be taken into account
- Practically there are two ways of doing this:
    a) Conservative approach: all uncertain parameters are chosen so as to obtain the worst results (from safety point of view) with a high degree of confidence
    b) Best-estimate plus uncertainty (BEPU) approach: all assumptions are made as realistically as possible, and the uncertainties of the code outputs are quantified using statistical methods
- Practically the conservative approach is still by far the most utilized way of performing deterministic safety analyses, but BEPU is gaining popularity

Summary

Summary

- Purpose of this lecture was to give an overview on how system-scale thermal-hydraulic simulation tools work
  - What the codes are based on (the fundamental physical principles, and flow models)
  - How the field equations are solved numerically, and what kind of numerical issues have to be dealt with when developing this kind of codes
  - How the closure laws are utilized, where they come from, and what are the limitations related to them
  - How the confidence in the results obtained with system-scale tools is established, what are the limitations of system-scale modelling
  - All of these are much larger subjects than can be covered in few hours

In a nutshell

- System-scale thermal-hydraulic codes are
  - Based on simplified description of physical phenomena, which sometimes forms a mathematically ill-posed problem (the macroscopic single-pressure two-fluid model)
    - These simplifications are necessary to be able to model complete power plants with the computer equipment available today (or during 1980's, when the system-scale tools started to mature. . .)
  - Contain a very large number of empirical correlations of sometimes questionable quality, that is often used way out of its intended parameter ranges. These closure laws compensate the loss of information caused by simplification of the field equations.
- Confidence in simulation results obtained with this kind of highly approximative simulation tools is established through a rigorous verification and validation process
  - The validation process is used to form an estimate on the uncertainties related to the code outputs. These uncertainties are then taken into account when applying the code for safety analysis purposes
  - The validation covers only the parameter ranges and situations encountered in the validation experiments.
  - **Extrapolation of the code use beyond the validation basis is thus generally not possible, or should be done with extreme care.**