A. Hoffmann, B. Merk, T. Hirsch and R. Pitz-Paal

Simulation of thermal fluid dynamics in parabolic trough receiver tubes with direct steam generation using the computer code ATHLET

In the present feasibility study the system code ATHLET, which originates from nuclear engineering, is applied to a parabolic trough test facility. A model of the DISS (Direct Solar Steam) test facility at Plataforma Solar de Almeria in Spain is assembled and the results of the simulations are compared to measured data and the simulation results of the Modelica library “DissDyn”. A profound comparison between ATHLET Mod 3.0 Cycle A and the “DissDyn” library reveals the capabilities of these codes. The calculated mass and energy balance in the ATHLET simulations are in good agreement with the results of the measurements and confirm the applicability for thermodynamic simulations of DSG processes in principle. Supplementary, the capabilities of the 6-equation model with transient momentum balances in ATHLET are used to study the slip between liquid and gas phases and to investigate pressure wave oscillations after a sudden valve closure.


1 Introduction

The parabolic trough technology with direct steam generation (DSG) (Fig. 1) is given. The main benefits of this technology compared to the mostly used heat transfer fluids are the high-
er efficiency, the lower investment and operating costs and less environmental impact in case of a pipe failure [1–2]. On the other hand, new challenging conditions occur in the DSG process which are mainly a two-phase flow of water and steam as well as high pressure conditions in the receiver pipe. In comparison to other technologies with heat transfer fluid, the DSG process uses parabolic trough collectors to concentrate sunlight on a receiver and to evaporate water directly in the receiver and finally to produce superheated steam which can drive a steam turbine and a generator for electricity production. The DSG process can be utilized in three different operation modes: recirculation-mode, once-through-mode and injection mode. The recirculation-mode has been thoroughly investigated at the DISS test facility at Plataforma Solar de Almeria in Spain [3–4]. Figure 2 shows the scheme of the DISS test facility.

In the recirculation-mode the collectors 1 to 9 with a combined length of \( l = 425 \) m are used to evaporate a part of the feed water until a certain steam quality is reached. Afterwards the water and steam phase are separated in the water/steam separator. Only the steam goes to collectors 10 and 11 (combined length of \( l = 75 \) m) for superheating. The leftover water feeds the inlet of the collector row by passing the recirculation pump. Typical operating conditions are from 35 bar/350°C up to 120 bar/500°C.

In the following, the scope of the present study is outlined. To predict the behaviour of the water/steam flow inside of the absorber pipes, numerical simulation tools are applied. Recently, this research has a specific interest in the investigation of flow instabilities which may occur in such a facility. The objective of the present study is to state the necessary prerequisites for a detailed analysis of flow instabilities in the future work. ATHLET Mod 3.0 Cycle A (Analysis of Thermal-hydraulics of LEaks and Transients) is chosen as simulation tool, due to its implemented transient momentum equation and comprehensive two-phase flow modelling which is an essential feature to study flow instabilities. Furthermore, it provides a different equation model compared to, for instance, the Modelica library “DissDyn” of the German Aerospace Center. All model assumptions of the “DissDyn” library and the ATHLET code are stated in a deeper manner and are compared in section 3. In section 4, the validation of ATHLET post-test calculations is conducted by checking the mass and energy balance with the results of measurements and the results of the “DissDyn” library. Moreover, a sudden valve closure is presented, calculated with ATHLET as transi-
ent test case which shows the propagation of pressure wave oscillations in section 5.

2 Review of literature

The following review provides information about conducted numerical simulations of the thermal hydraulics in line-focused parabolic trough power plants with direct steam generation. It will be discussed which model assumptions have been used in previous tools and which investigations have been already conducted with regard to flow instabilities.

Most of the applied numerical models are based on the homogeneous equilibrium model which principally assumes no slip thermodynamic equilibrium between the both phases [5–10], however the two-phase flow is probably not well mixed at all positions along the absorber pipe [11]. Furthermore by default, mass, momentum and energy balance are used to describe the fluid flow and an additional energy equation treats the absorber wall [5–8, 12]. Only a few studies [6, 7, 13] have been conducted with a transient momentum equation despite the crucial importance of time-dependent effects of fluid dynamics during the operation of a solar thermal power plant with DSG process under real conditions.

A steady state momentum equation and the homogeneous equilibrium model have been used by Lippke [5, 14] and Hirsch [8, 15]. Both investigations are related to the control of the fluid flow. Hirsch developed a Modelica model for the software package Dymola which enables a connection of fluid flow and control components in one tool (cf. section 3.1). The main objective has been the understanding of the effects of control schemes on the plant operation. Further research has been performed by Moya et al. [12] and Lobón et al. [9] on steady state results of the DISS test facility sited at Plataforma Solar de Almería. Moya et al. have focused on the flow pattern, the heat transfer coefficients and the wall temperatures which have been calculated with the RELAP software package. RELAP has comparable features like ATHLET which is used in the present study. In contrast, Lobón et al. used the three-dimensional computational fluid dynamic package STAR-CCM+ to compare the calculated steam fractions, fluid temperatures and pressures with the results of the measurements.

Odeh et al. [6, 16] and Steinmann [7] developed numerical tools which treat the momentum equation in a transient manner which is an important prerequisite for studying time-dependent behaviours of the fluid flow. Odeh et al. performed simulations regarding the influence of changing radiation conditions on the exit temperature. Steinmann investigated transient flow conditions along the whole pipe and studied flow instabilities of solar thermal power plants in once-through mode for the first time. The research included the investiga-
tion of the Ledinegg instability as well as dynamic instabilities for a single pipe and the parallel pipe instability for two parallel pipes. This study proves that the Ledinegg instability can be avoided with an orifice before the first absorber pipe or a inlet temperature with a low subcooling into the first absorber pipe. For the dynamic instabilities the choice of the boundary conditions is essential for a stable or unstable flow condition. His results showed no oscillations in the velocity when the enthalpy and the mass flow are given at the inlet and the pressure is given at the outlet. Parallel pipes revealed instabilities as well which can be avoided with a control valve at each pipe inlet for a hydraulic decoupling of the pipes [7].

The direct steam generation process is well investigated with a steady momentum equation and the homogeneous equilibrium model and is partly investigated with a transient momentum equation and the homogeneous equilibrium model. But there are numerical tools available which provide separated conservation laws for the liquid and gas phase as well as a transient momentum equation. Therefore, in the present study the ATHLET code is applied which is a common numerical simulation tool in the field of the reactor safety analysis. The selected ATHLET code enables to install control systems and can be applied to non-nuclear systems as well. Therefore, this tool mainly combines separated conservation laws, a transient momentum equation and a coupling of control system and fluid dynamics within one code. These features enable to get more information about the behaviour of the fluid flow and to conduct a detailed analysis of potential flow instabilities which can not sufficiently be represented by simplified approaches.

3 Computer codes for thermal-hydraulics

For a clear distinction between the capabilities of the “DissDyn” library and the ATHLET code the model equations and assumptions are compared and discussed.

3.1 Modelica library Dissdyn

The Modelica library “DissDyn” has been developed by Hirsch [8, 15] for internal use at the German Aerospace Center and can be included in the software package Dymola – Dynamic Modeling Laboratory [17]. Dymola is a multi-engineering modeling and simulation tool which uses Modelica models as basis. The modelling for a physical system is made with the object-oriented language Modelica. The provided “DissDyn” library allows the assembly of a fluid system of a parabolic trough collector with DSG process within Dymola.

3.1.1 Conservation laws

\[ \frac{\partial p}{\partial t} + \frac{\partial}{\partial x}(\rho u) = 0, \]  
\[ \frac{\partial p}{\partial x} = \rho \frac{\partial u}{\partial x} = \frac{\rho}{V} \frac{\partial Q}{\partial t}. \]

The main task of the “DissDyn” library is the description of the fluid dynamics of the two-phase flow in the receiver. The one-dimensional conservation laws of mass, momentum and energy are stated as follows:

Eq. (2) displays that the momentum equation has been reduced to a stationary equation for frictional pressure losses. Furthermore, these equations assume mechanical and thermal equilibrium in the two-phase flow, i.e. a mixture velocity and mixture properties are defined. To obtain de-coupled equations for the description of the state in each control volume the pressure and the specific enthalpy have been chosen as state variables. In this way two explicit equations in the time derivatives of pressure and specific enthalpy are found by reshaping of mass and energy equation of the fluid.

Supplementary to the conservation laws of the fluid a further energy equation is used to describe the heat conduction in the receiver pipe wall

\[ A_{stop} c_p \frac{\partial T_w}{\partial t} = \dot{Q}_{in} - \dot{Q} \]  

with the rate of heat flow \( \dot{Q}_{in} \) into the absorber pipe and the rate of heat flow \( \dot{Q} \) from the wall into the fluid in units of [W/m].

3.1.2 Closure equations

One closure equation is the pressure loss correlation proposed by Müller-Steinhagen et al. [18]. This correlation provides \( \Delta p \) as explicit function depending on mass flow \( \dot{m} \) and flow quality \( \dot{x} \). Another important closure equation determines the heat flux

\[ \dot{Q} = \alpha_{HTC} \pi d(T_w - T_R) \]

between wall and fluid. The heat transfer coefficient \( \alpha_{HTC} \) is calculated by the Dittus-Boelter equation [19] in the single phase region and can be calculated with a boiling heat transfer approach in the two-phase region. However, studies revealed that the dynamics of the evaporator are well reproduced by a constant heat transfer coefficient of \( \alpha_{HTC} = 10000 \text{ W/m}^2 \).

3.1.3 Further assumptions and capabilities

The state variables are used to compute the required fluid properties such as steam fraction, mixture density, temperature as well as dynamic viscosity, specific heat capacity, heat conductivity and surface tension for the liquid and the gas phase. The range of validity of the exploited functions to determine the fluid properties is shown in Table 1.

As boundary conditions the mass flow and the specific enthalpy are given at the inlet and the pressure is given at the outlet of the system configuration. All pipes are spatially discretized by using the finite-volume approach.

Specific models are inserted to match the needs of the solar thermal power plants. There are models included for components such as liquid pools, water/steam separators, valves and pumps. The energy supplied by the sun is transferred into an external heat flux \( \dot{Q}_{ext} \) which can be set as boundary condition for the receiver pipes and appears in Eq. (4). Thereby, several influences on the final heat flux are taken into account such as sun position depending on the day of the year and the time of day, the geographical latitude and the altitude based on the position of the facility, cloud coverage and the defocussing of the collector, the magnitude of direct irradiation as well as the efficiency of the collector.

To introduce a control system, the connected Modelica library brings along features that are able to add a variety of control components to the system. Also the entire process of numerical integration is utilized by the Dymola software.
Table 1. Range of validity of water-steam properties package in “DissDyn” and ATHLET

<table>
<thead>
<tr>
<th>Property</th>
<th>Range of validity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Modelica library “DissDyn” [13]</td>
<td>Pressure: $3.0 \cdot 10^5 \text{ Pa} \leq p \leq 1.2 \cdot 10^7 \text{ Pa}$</td>
</tr>
<tr>
<td></td>
<td>Temperature: $100.0^\circ\text{C} \leq T \leq 500.0^\circ\text{C}$</td>
</tr>
<tr>
<td>ATHLET [23, 1]</td>
<td>Pressure: $1.0 \text{ Pa} \leq p \leq 2.2 \cdot 10^7 \text{ Pa}$</td>
</tr>
<tr>
<td></td>
<td>Temperature: $-40.0^\circ\text{C} \leq T \leq 371.85^\circ\text{C} (\text{liquid})$</td>
</tr>
<tr>
<td></td>
<td>$-270.0^\circ\text{C} \leq T \leq 6000.0^\circ\text{C} (\text{steam})$</td>
</tr>
</tbody>
</table>

The validation of the “DissDyn” library has been done with analytical solutions of certain cases and experimental data which was gathered at the DISS test facility at Plataforma Solar de Almería. In general, the “DissDyn” library offers proper features for solar thermal power plants and its application to the DSG process with recirculation-mode is proven [15].

3.2 ATHLET

ATHLET (Analysis of THermal-hydraulics of LEaks and Transients) is a lumped-parameter simulation code developed by the Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) mbH [19–22]. The field of application is primarily aligned to light water reactors. For instance the analyses are with regard to abnormal plant transients, leaks or other types of incidents in a nuclear power plant. But ATHLET is also capable of treating topics which are not connected to nuclear engineering [21].

ATHLET consists of several modules which are: “Thermo-fluidodynamics”, “Heat Transfer and Heat Conduction”, “Neutron Kinetics” and “General Control Simulation Module” (GCSM) [21]. The two first-mentioned modules are the most important ones for the present study. A deeper view into these modules is given. Furthermore, FEBE (Forward-Euler, Backward-Euler) is an essential part of the software which solves the first-order ordinary differential equations.

3.2.1 Conservation laws

The “Thermo-fluidodynamics” module is the basic component of ATHLET which provides the one-dimensional partial differential equations of the fluid dynamics. It has a 5-equation and a 6-equation model. The 5-equation model uses a mass and energy equation separately for the liquid and the vapor phase and a momentum equation with mixture properties of the two-phase flow combined with a Drift-Flux model. In the 6-equation model (two-fluid model) the conservation law for momentum is stated separately for the liquid and the vapor phase [19]. The mass balances are

$$\frac{\partial}{\partial t}((1-\alpha)\rho_l) + \frac{\partial}{\partial x}((1-\alpha)\rho_l \dot{\omega}_l) = -\nabla,$$  

(6)

$$\frac{\partial}{\partial t}(\alpha \rho_v) + \frac{\partial}{\partial x}(\alpha \rho_v \omega_v) = \nabla$$  

(7)

for the liquid and the vapor phase respectively. The 6-equation model provides a separated momentum equation

$$\frac{\partial}{\partial t}((1-\alpha)\rho_l \dot{w}_l) + \frac{\partial}{\partial x}((1-\alpha)\rho_l \dot{w}_l^2) + \frac{\partial}{\partial x}(1-\alpha)\rho_l \dot{w}_l = \tau_l - (1-\alpha)\tau_w - \nabla \omega_l + (1-\alpha)\rho_l \dot{g} + S_{M,l},$$  

(8)

$$\frac{\partial}{\partial t}(\alpha \rho_v \dot{w}_v) + \frac{\partial}{\partial x}(\alpha \rho_v \dot{w}_v^2) + \frac{\partial}{\partial x}(\alpha \rho_v \dot{w}_v) = -\tau_v - \alpha \tau_w + \nabla \omega_v + \alpha \rho_v \dot{g} + S_{M,v},$$  

(9)

for the liquid and the vapor phase respectively. The first term on the right hand side takes into account the interfacial shear forces, the second term the wall shear forces, the third term the momentum flux due to phase change, the fourth term the gravitational forces and terms $S_{M,l}$ and $S_{M,v}$ summate external momentum sources like a pump. To complete the 6-equation model two energy equations for the liquid and the vapor phase are defined as follows

$$\frac{\partial}{\partial t} \left( (1-\alpha)\rho_l \left( h + \frac{w_l^2}{2} \right) \right) + \frac{\partial}{\partial x} \left( (1-\alpha)\rho_l \dot{w}_l \left( h + \frac{w_l^2}{2} \right) \right) = -p \frac{\partial}{\partial t} (1-\alpha) \frac{\dot{Q}_l}{V} + \frac{\dot{Q}_l}{V} + \nabla \left( h + \frac{w_l^2}{2} \right) + S_{E,l},$$  

(10)

$$\frac{\partial}{\partial t} \left( \alpha \rho_v \left( h_v + \frac{w_v^2}{2} \right) \right) + \frac{\partial}{\partial x} \left( \alpha \rho_v \dot{w}_v \left( h_v + \frac{w_v^2}{2} \right) \right) = -p \frac{\partial}{\partial t} \frac{\dot{Q}_v}{V} + \frac{\dot{Q}_v}{V} + \nabla \left( h_v + \frac{w_v^2}{2} \right) + S_{E,v},$$  

(11)

with $\dot{w}_l = \omega_l$ for condensation and $\dot{w}_v = \omega_v$ for evaporation. In the energy equation the first term on the right hand side compensates a part of the time derivation from the left hand side. The second term on the right hand side considers the heat flow through structures, the third term the heat flow at the phase interphase, the fourth term the energy flux due to phase change and the fifth term other external sources. The fractions of dissipation mechanisms and the potential energy are neglected, because of their small magnitude compared to an external heat source and the enthalpy fluxes [9, 23].

The conservation laws in this manner enable the ATHLET code to take into account the thermal and mechanical non-equilibrium. Similar to the Modelica model an energy balance for modelling of the heat conduction in solid materials is provided by the ATHLET code in the module “Heat Conduction and Heat Transfer”.

The energy balance for one heat conductor layer with the volume $V$ is defined as follows:

$$V \frac{\partial}{\partial t} \dot{T}_w = Q_{ext} - \dot{Q} + S_{heat}$$  

(12)

where the heat flow $\dot{Q}$ and $Q_{ext}$ is used in units of [W]. The last term on the right hand side represents an additional volume heat source in the layer. The heat conductor module enables a two-dimensional discretization in the radial and the axial direction. But only the one dimensional energy equation

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in radial direction is solved for the wall elements; the axial heat conduction is not taken into account.

3.2.2 Closure equations

The modelling of the frictional pressure loss in the two-phase region is done by applying the pressure loss correlation of Martinek and Nelson [24] or Chisholm [25] in the 6-equation model. The 5-equation model offers even more models for the pressure losses due to friction which are not discussed in the present study because of the exclusive usage of the 6-equation model. In the two-fluid model the frictional pressure losses are calculated separately

\[ \Delta p_l = \zeta_w \frac{\rho_l}{2} w_l |w_l| \]  
(13)

\[ \Delta p_r = \zeta_w \frac{\rho_r}{2} w_r |w_r| \]  
(14)

for the liquid and the steam phase respectively. The aggregated pressure loss of Eq. (13) and Eq. (14) obtains already the influence of changing mixture density depending on steam quality [19]. The additional pressure drop in the two-phase region is considered by a two-phase multiplier \( C_p \). But due to the separate calculation of the pressure drop for the liquid and the steam phase the original two-phase multiplier \( C_p \) of either the Martinelli and Nelson correlation or the Chisholm model is modified as follows:

\[ C_p^* = C_p \cdot \frac{\rho_m}{\rho_l} \]  
(15)

within the ATHLET code in the 6-equation model. The determined pressure drop for the liquid and the steam phase is multiplied with \( C_p^* \) and is inserted in the momentum balances Eq. (8) and Eq. (9) respectively. Other irreversible pressure losses are form pressure losses in e.g. bends, branches or contractions of the flow path which can be taken into consideration by a separate input of form loss coefficients at the desired position.

A further feature of the module "Heat Conduction and Heat Transfer" is exploited for the determination of the heat transfer coefficient between wall and fluid in single phase and two-phase flow. This module provides several correlations depending on the heat transfer regime. ATHLET considers the following four heat transfer levels [19]:

- Heat flow from fluid to wall (natural and forced convection, film condensation),
- Heat flow from wall to fluid (natural and forced convection, subcooled and saturated nucleate boiling),
- Transition boiling,
- Film boiling.

ATHLET calculates the distribution of the total heat flux to the liquid and the steam phase. Therefore, the case can be considered that the direction of the heat flow to the liquid and the steam phase is opposite. In that case only the heat flux which is consistent with the total heat flux is taken into account.

During evaporation and condensation a momentum exchange exist between the phases. This momentum exchange is described by the interphase mass exchange \( \psi \) which enters mass, momentum and energy balances. The interphase mass exchange \( \psi \) plays an important role for the magnitude of the thermodynamic non-equilibrium during evaporation and condensation. ATHLET provides specific models for the determination of the interphase mass exchange when evaporation or condensation occurs [19].

A term for the interfacial shear appears in the momentum balances. The magnitude of the interfacial shear forces is heavily influenced by the existing flow pattern. Hence, ATHLET includes a model for the determination of the flow pattern in vertical and horizontal pipes. Once the flow pattern is known an interfacial shear stress coefficient \( C_t \) is calculated by correlations. The interfacial shear stress is described with the interphase perimeter \( P_l \) as follows:

\[ \tau = \frac{A}{P_l} C_t w_r^2 \]  
(16)

This interfacial shear depends on the relative velocity between both phases and expresses either the transport of momentum from the steam phase to the liquid phase or vice versa. The total momentum of the flow is conserved.

3.2.3 Further assumptions and capabilities

There are different water-steam properties packages included in ATHLET. The used water-steam propylene package has been proposed by Müller [26]. The range of validity is given in Table 1. There are two types of boundary conditions which are either a pressure or a mass flow boundary condition. A so called once-through system has a mass flow boundary condition at the inlet and a pressure boundary condition at the outlet or vice versa depending on the application. Further boundary conditions like the heat flow into the absorber pipe are determined externally and are entered directly in ATHLET. In general, there are no specific models for solar thermal power plants in the ATHLET code.

The basic module GCSM plays an important role in ATHLET. It can be used to model an entire balance-of-plant system and other control circuits. Besides, it enables a direct interaction between thermal-hydraulics and control components and can be used to control boundary conditions during a time dependent calculation.

As described in section 3.2.1, the "Thermo-fluidynamics" module is a main module in ATHLET. It supplies the so called thermo-fluidodynamic objects which can be e.g. a pipe object or a branch. They can be used to build a system configuration. The objects are divided into control volumes for the spatial discretization of the fluid domain. For the discretization of the balance equations a staggered grid approach is adopted, calculating the scalar quantities at the cell centers and the velocities at the faces of the control volumes. In addition, special objects like pumps, condensators, valves and steam turbines can be represented in ATHLET.

Important prerequisites for a successful application on solar thermal power plants are fulfilled. Furthermore, it is worth to mention that ATHLET has undergone a broad validation, but mostly related to its application in nuclear reactor safety [22].

3.3 Comparison between both computer codes

The brief descriptions of the "DissDyn" library within Dymola and the ATHLET code pointed out the different origins of both software packages and their underlined equations and correlations. Table 2 summarizes the comparison results for both tools of the most important features.

Table 2 also shows the different assumptions for the conservation laws. Especially the transient momentum equation and calculation of the slip between liquid and gas phase in ATHLET exceed the abilities of the "DissDyn" library. The ATHLET code considers much more mechanisms in the momentum balance like interfacial shear forces and momentum
forces due to evaporation and takes into account additional effects in the energy balance like energy flow due to phase change and heat flow at the phase interface.

For the pressure drop calculation different correlations are used in the “DissDyn” library and the ATHLET code. In previous numerical investigations Steinmann [7] and Odeh [6] used the pressure drop correlation of Martinelli and Nelson [24], but they did not verify this correlation with measurements of the pressure loss of a solar thermal power plant with DSG. Lippke [5] used the Friedel correlation [27] in combination with the Beattie correlation [28] which was proposed by Kastner et al. [29]. For the “DissDyn” library Hirsch [15] compared experimental data of the DISS test facility with different pressure loss correlations. Therefore, the Friedel correlation suited the experimental data very well, but due to implementation constrains the Müller-Steinhagen correlation was chosen.

The determination of the heat flow from the wall to the fluid is made in the “DissDyn” library with the Dittus-Boelter equation [19] in the single phase region and a fixed heat transfer coefficient in the two-phase flow. In comparison ATHLET adjusts the correlation of the heat transfer coefficient depending on the flow conditions. So there are a lot of heat transfer correlations implemented in ATHLET which cover a wide range of heat transfer regimes.

It is noteworthy that the “DissDyn” library provides a suitable conversion of the direct normal irradiance onto parabolic trough collectors into a heat flux onto the receiver pipe. ATHLET needs a pre-calculation of the heat flux as input parameter.

4 Post-test calculations with ATHLET

4.1 Model of DISS test facility in ATHLET

The DISS test facility at Plataforma Solar de Almería (Fig. 2) is the object of investigation. This facility is modelled with ATHLET.

All eleven absorber pipes of Fig. 2 with a combined length of 500 m, the connection pipes in between and a vertical pipe as water/steam separator are assembled in ATHLET. Table 3 gives an overview of the geometrical configuration. Figure 3 shows the created ATHLET model.

<table>
<thead>
<tr>
<th>Physical models and assumptions</th>
<th>Modelica library “DissDyn” within Dymola</th>
<th>ATHLET</th>
</tr>
</thead>
<tbody>
<tr>
<td>Momentum equation</td>
<td>- stationary</td>
<td>- transient</td>
</tr>
<tr>
<td></td>
<td>- one equation for mixture flow</td>
<td>- liquid/gas phase separately (6-equation model)</td>
</tr>
<tr>
<td></td>
<td>- mechanical equilibrium</td>
<td>- or mixture flow (5-equation model + drift-flux model)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>- mechanical non-equilibrium</td>
</tr>
<tr>
<td>Mass equation</td>
<td>- one equation for mixture flow</td>
<td>- two equations liquid/gas phase separately</td>
</tr>
<tr>
<td>Energy equation</td>
<td>- one equation for mixture flow</td>
<td>- two equations liquid/gas phase separately</td>
</tr>
<tr>
<td></td>
<td>- thermal equilibrium</td>
<td>- thermal non-equilibrium</td>
</tr>
<tr>
<td>friction</td>
<td></td>
<td>6-equation model</td>
</tr>
<tr>
<td></td>
<td></td>
<td>- further models 5-equation model</td>
</tr>
<tr>
<td>Heat transfer correlation</td>
<td>- Dittus-Boelter equation [32] (single phase region)</td>
<td>- correlation depends on heat transfer regime [1]</td>
</tr>
<tr>
<td></td>
<td>- ( \alpha = 10000 \text{ W/m}^2 \text{ = const. (two-phase region)} )</td>
<td></td>
</tr>
<tr>
<td>Heat conduction in receiver</td>
<td>- no axial heat conduction</td>
<td>- no axial heat conduction</td>
</tr>
<tr>
<td>wall</td>
<td>- no radial discretization</td>
<td>- radial discretization</td>
</tr>
<tr>
<td></td>
<td>- no azimuthal discretization</td>
<td>- and three material layers possible</td>
</tr>
<tr>
<td></td>
<td></td>
<td>- azimuthal discretization by using GCSM</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Component</th>
<th>( l ) in m</th>
<th>( d_1 ) in mm</th>
<th>( d_e ) in mm</th>
<th>Number of 90 degree bends</th>
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</thead>
<tbody>
<tr>
<td>Collector 1–8 and 11</td>
<td>50</td>
<td>50</td>
<td>70</td>
<td>0</td>
</tr>
<tr>
<td>Collector 9 and 10</td>
<td>25</td>
<td>50</td>
<td>70</td>
<td>0</td>
</tr>
<tr>
<td>Connection pipe between collector 1–8</td>
<td>11</td>
<td>59</td>
<td>73</td>
<td>8</td>
</tr>
<tr>
<td>Connection pipe between collector 8 and 9</td>
<td>17</td>
<td>59</td>
<td>73</td>
<td>8</td>
</tr>
<tr>
<td>Connection pipe between collector 9 and separator</td>
<td>49</td>
<td>59</td>
<td>73</td>
<td>8</td>
</tr>
<tr>
<td>Connection pipe between separator and collector 10</td>
<td>50</td>
<td>59</td>
<td>73</td>
<td>11</td>
</tr>
<tr>
<td>Connection pipe between collector 10 and 11</td>
<td>11</td>
<td>59</td>
<td>73</td>
<td>8</td>
</tr>
<tr>
<td>Separator</td>
<td>( \approx 3 )</td>
<td>1300</td>
<td>1450</td>
<td>0</td>
</tr>
</tbody>
</table>
To compare the ATHLET results against calculations from the “DissDyn” library an opened fluid cycle model is chosen, i.e. recirculation pump, feedwater pump and balance of plant are cut out of the model and are represented by boundary conditions. At the inlet the mass flow $\dot{m}$ (Fig. 5) and the specific enthalpy $h$ are given as boundary conditions and the pressure $p$ is given as boundary condition at the outlet. A further mass flow boundary condition is given for the separated water in the water/steam separator which simulates the recirculation pump.

The slope of the terrain at Plataforma Solar de Almería is considered in the model. To achieve a completely horizontal receiver, each connection pipe is taken into account a difference in the altitude of $\Delta l = 0.8$ m between collector 1 and 8 and $\Delta l = 0.4$ m between collector 8 and 10. According to the geometry a lot of 90 degree bends as well as contractions and expansions of the flow path appear in the pipe system (Table 3). Form loss coefficients are introduced to determine a proper pressure loss at these positions along the pipe.

Besides the geometrical specification, the 6-equation model and Martinekli and Nelson pressure loss correlation are applied. The effective heat flux onto the receiver is calculated outside of ATHLET and is included by a heat conduction object as homogeneous heating of the outer absorber pipe surface, i.e. the tube is heated uniformly and no directional dependence of the heat source is considered. Each absorber pipe, connection pipe as well as the water/steam separator is connected to a heat conduction object which is spatial discretized by 10 layers with equal thickness. The material of all heat conduction objects is steel with a density $\rho = 7600$ kg/m$^3$, a thermal conductivity $\lambda = 38$ W/mK and a specific heat capacity $c_p = 540$ J/kgK. The heat conduction object is additionally used for the representation of the heat losses of the system. The determination of heat losses is a complicated task especially for the connection pipes. Therefore, a simplified approximation of the heat losses is used, so that an accurate steady state condition is achieved (Fig. 7). The spatial resolution follows similar values in the literature with a minimum of one control volume per $\Delta x = 5$ m [8, 12]. A test calculation with a finer resolution in ATHLET showed no differences in the simulation results.

4.2 Results and discussion

This study conducts simulations with ATHLET besides the originally field of application of this code. To evaluate the abilities of the ATHLET code in the field of direct steam generation in parabolic trough collectors a comparison with measured data and the “DissDyn” library is performed. Hence, both software packages are applied for the same test case.

One hour of operation under real conditions at DISS test facility is chosen as test case. The measurements have been carried out on 2000-06-16 between 18:00 and 19:00. The objective of the test case is to study the transient plant behaviour during a sudden pressure decrease after collector 11. This test case can fulfill the purpose of the investigation which is to prove the applicability of ATHLET onto such facilities. It also has been simulated a test case with a sudden mass flow decrease at the inlet and a test case with real irradiation disturbances during a day which are both not presented in this study.

Figures 4 and 5 show two of the implemented boundary conditions in ATHLET and the “DissDyn” library. Additionally, the specific enthalpy at the inlet of absorber pipe 1, ambient temperature with $T = 25$°C, a constant recirculation mass flow at the water/steam separator and solar irradiance as heat flux into the receiver pipe are given. The heat input is linearly decreasing from $Q = 3015$ W/m to $Q = 2722$ W/m from $t = 18.0$ h to $t = 19.0$ h. These boundary conditions are applied analogous to both software packages. There are no differences in the boundary conditions. The ATHLET simulations are computed in parallel on the dual-core processor AMD Athlon II X2 265 with 3.30 GHz. This processor enables the calculation of one hour of operation at the DISS test facility in a CPU time of $t_{CPU} = 28$ min.

Figures 6, 7 and 8 present the results of three calculated fluid dynamic parameters of the above mentioned test case. The selected fluid dynamic parameters are used for the com-

![Fig. 3. Scheme of assembled model of DISS test facility in ATHLET and necessary boundary conditions at inlet, outlet and water/steam separator](image-url)
parison between the measured data, the “DissDyn” library and the ATHLET code. These variables permit to assess the performance of the simulation tools.

Figure 6 shows the calculated and the measured mass flow of steam at the outlet of absorber pipe 11. The reached steady state case of ATHLET at \( t = 18.0 \) h matches the determined mass flow at the DISS test loop. Also the dynamic behaviour of the mass flow due to the pressure decrease can be properly calculated by ATHLET. Only the mass flow oscillations after \( t = 18.8 \) h are not represented due to the simplified pressure boundary condition, see Fig. 4. The Modelica results of the outlet mass flow in Fig. 6 differ slightly from the steady state case at \( t = 18.0 \) h. Thus, steady state conditions at the beginning of the simulation are probably not fully reached. In the dynamic behaviour it can be seen that the mass flow in the Modelica model responds stronger during changing conditions compared to the ATHLET calculation. The missing consideration of the slip in the Modelica model could be an explanation which has to be confirmed in further research. The smooth curves in the results of both simulation tools compared to the measurement follow from the simplified boundary conditions which does not represent small fluctuations.

The steam temperature at the outlet of receiver pipe 11 is well calculated by ATHLET and Modelica “DissDyn” (Fig. 7).

There is a slight difference in the absolute value of the ATHLET and “DissDyn” calculation which can be explained with the simplified heat loss assumptions. Between \( t = 18.0 \) h to \( t = 18.1 \) h it can be seen that the steam temperature of “DissDyn” is moving towards the final steady state condition. This finding is consistent with the plot of the steam mass flow \( t = 18.0 \) h (Fig. 6). The dynamic behaviour is well predicted by ATHLET. The steam temperature of “DissDyn” reacts stronger during changing conditions and shows steeper gradients and higher local extrema. Possible reasons for that could be the differences in the heat transfer coefficient or the representation of the pipe wall. Further research is necessary in this field.

Figure 8 depicts the calculated inlet pressures of both simulation tools which agree well with the measured data. But the calculated pressures are displayed with an offset in Fig. 8. These deviations are connected to the difficulty of the prediction of the frictional pressure drop for a two-phase flow by a pressure drop correlation. The magnitude of the level correction implies the deviation to the measured pressure drop between inlet and outlet of the DISS test facility. ATHLET clearly overestimates the overall pressure loss and “DissDyn” underestimates the overall pressure loss. The largest fraction of the overall pressure loss is due to friction in the ATHLET calculation. The Darcy-Weissbach friction factor \( \lambda_2 \) is calculated within ATHLET depending on the Reynolds number...
by assuming a rough pipe with a wall roughness of 0.06 mm. It is used for laminar flow the Hagen–Poiseuille equation and for turbulent flow the Colebrook correlation. ATHLET also considers bends and extractions and contractions of the flow path with extra form loss coefficients. The overall pressure drop due to these form loss coefficients is $\Delta p = 0.8$ bar. The results of the Modelica calculation give a lower prediction of the overall pressure loss for a smooth pipe with the Müller–Steinhagen correlation, but match the trend of the measured pressure clearly better than ATHLET (Fig. 8). One reason for these deviations is the assumption of a rough pipe in ATHLET and a smooth pipe in Modelica. Nevertheless, there will be further studies carried out to find a proper correlation for the two-phase frictional pressure loss in solar thermal power plants with DSG.

There are some topics which require further research. But the overall mass and energy balance of one specific case are sufficiently accurate predicted by the ATHLET code and the “DissDyn” library. The two further test cases which are not presented here, confirm this agreement. Furthermore, the measurement errors should be considered. The mass flow is determined with a measurement error of $\Delta m = 0.045$ kg/s at the DISS test loop. The uncertainties for the pressure measurements are within $\Delta p = 0.9$ bar and for the temperature measurements within $\Delta T = 4$ K.

Besides the comparison, additional information about the DSG process is collected which has not been measured during the experiment and cannot be calculated with the Modelica model. Hence, the slip

$$s = \frac{w_r}{w_l}$$  \hspace{1cm} (17)

is calculated out of the results of the ATHLET code. The slip is mainly caused by the pressure gradient along the pipe which counteracts the force of the momentum exchange between the liquid and the steam phase due to different velocities of the phases [30].

The differences in the velocity of steam and liquid phase along the receiver pipe are shown in Fig. 9. Three different positions along the two-phase region are selected. The positions $x = 0$ m and $x = 500$ m refer to the inlet at receiver pipe 1 and the outlet of receiver pipe 11, respectively, without counting the length of the connection pipes in between. From the calculated velocities can be seen that there is a noteworthy slip between the steam and the liquid phase. The maximum slip is found at position $x = 202.5$ m with $s \approx 2$, i.e. the gas phase precedes the liquid phase with twice the velocity. The different values for the slip at different positions reveal the magnitude of the influence between the both phases. Furthermore, the acceleration of both phases from the beginning of the two-phase flow to the position $x = 402.5$ m can be seen in Fig. 9. The reason for the slip and the different acceleration of the phases is the difference in the densities of the liquid and the steam phase [30]. In principal, the more steam is produced, the higher must be the velocity to fulfill the conservation laws. Additional, the gas phase accelerates the liquid phase as well. Figure 9 illustrates the effect of the pressure decrease at the outlet of absorber pipe 11. The closer the outlet is, the stronger is the impact on the velocities of the liquid and the steam phase.

The slip plays an important role in the determination of the two-phase pressure drop, because in a two-phase flow additionally to the wall friction there are pressure losses due to the momentum exchange between both phases. This effect is captured with the two-phase multiplier of the Martinelli and Nelson pressure drop correlation and therefore the real value of the slip does not influence the pressure drop calculation during the simulation. But the interfacial shear forces in Eq. (16) are obviously based on the slip and are considered in the momentum balances Eq. (8) and Eq. (9) so that there is a direct influence of the dynamic flow behavior due to the slip. Consequently, the slip might play an important role for the investigation of flow instabilities which will be performed with ATHLET in future work.

One has to keep in mind that the present study presents only one numerical calculation for one specific test case which shows only small deviations in the results of the “DissDyn” library and the ATHLET code. But much more investigations are necessary in order to make a statement about the most valuable modelling approach. For the specific test case the 3-equation and the 6-equation approach seem to be equivalent. But the universal validity of this equivalence is not proven at the present state. There might be test cases which have effects that are not catchable with a 3-equation model and a 6-equation approach is necessary. Moreover, a proper validation of especially the simulated fluid velocities of the steam and the liquid phase in ATHLET requires an improved measurement technique with a higher spatial resolution.

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**Fig. 8. Pressure at the inlet of collector 1**

**Fig. 9. Steam and liquid velocity at different positions along the two-phase region**
5 Valve closure

In the following, a brief outlook is given about further work which is directed towards flow instabilities in solar thermal power plants with DSG process. There are a variety of possible flow instabilities like density wave oscillations and pressure wave oscillations which may occur in a single channel facility or parallel channel instabilities in an upscaled power plant with several parallel receivers. ATHLET provides excellent prerequisites for such studies. Several previous studies [31–33], conducted in the field of nuclear engineering, have confirmed these capabilities of ATHLET. Mainly the transient momentum equation enables ATHLET to investigate flow instabilities. Furthermore, the feedback between a control system and the thermal-fluid dynamics can be studied and modelled due to the GCSM in ATHLET.

The capabilities of ATHLET are exploited in a test case which demonstrates the occurrence of pressure wave oscillations. In the test case a valve closure is conducted in the feedwater pipe of a solar thermal power facility. The used ATHLET model depicts a facility in the once-through mode. Compared to Fig. 3 the water/steam separator is not included in the model, but all receiver pipes are taken into account. The feedwater pipe length between the inlet boundary condition and the first absorber is about \( l = 100 \) m. The valve is located in the single phase region in the feedwater pipe at 8 m upstream of the inlet of receiver tube 1. During steady state conditions this valve is closed suddenly. The spatial resolution and maximal temporal resolution is increased to \( \Delta x = 0.2 \) m and to \( \Delta t = 0.01 \) s, respectively, to achieve a proper prediction of the pressure wave oscillation. ATHLET automatically reduces the time step size on when it is required. Figure 10 displays the pressure wave oscillations downstream of the valve position. At two different positions the damped pressure wave oscillations occur almost at the same time. The reason for that is the propagation of pressure waves with the speed of sound and not with the velocity of the fluid which is a characteristic of pressure wave oscillations.

This brief outlook confirms the abilities of ATHLET for one kind of flow instabilities, but the result is not validated with experimental data. Still, the occurrence of pressure wave oscillations after a fast closure of a valve is a well-known problem in the field of piping construction. The test case indicates the possible pressure increase in a solar thermal power plant which is important for a proper construction of the components of the facility. Further research will estimate the potential of occurrence of flow instabilities for the specific application of a solar thermal power plant with DSG. All flow instabilities in the classification of flow instabilities of Bouré et al. [34] are evaluated. Afterwards interesting flow instabilities will be simulated with ATHLET.

6 Conclusions

This study shows results of numerical simulations with the DISS code of the fluid dynamics of a solar thermal test facility with direct steam generation.

ATHLET is compared to a second simulation tool which uses the “DissDyn” library within the Dymola environment. The differences in the model assumptions are discussed in detail. The “DissDyn” library uses the approach of a 3-equation system for the mixture flow. Instead, ATHLET uses two equations for each conservation law, i.e. one for the liquid phase and one for the gas phase. Additionally, ATHLET treats the momentum equation in a transient manner compared to the “DissDyn” library. Besides, both simulation tools use different correlations for the determination of the pressure drop in the two-phase region and the heat transfer coefficient.

The assembled ATHLET model of the DISS test loop at Plataforma Solar de Almería is able to predict the overall mass and energy balance of a selected test case appropriately. For this test case, the differences between the results of “DissDyn” library, the results of the ATHLET code and the plant data are small, except of the calculated pressure losses which requires further research. This specific result cannot prove whether a 3-equation approach or a 6-equation model is a satisfactory modelling option for all possible plant behaviours of a solar thermal power plant with DSG process. Other test cases may show larger deviations between these models, perhaps because of the slip plays a larger role.

Finally, the obtained results confirm the applicability of ATHLET for thermodynamic simulations of DSG processes and it has been shown that ATHLET enables a more detailed analysis of the evaporation process. The calculated slip between the liquid and the steam phase can be helpful to improve the understanding of the process at all. As a demonstration for upcoming studies, ATHLET’s Two-Fluid-model based on the fully time-dependent balance equations is used for the prediction of pressure wave oscillations after a sudden valve closure.

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Nomenclature

A Surface
Cp Specific heat capacity
Cp' Two-phase multiplier
Cp'' Modified two-phase multiplier
d1 Outer diameter
d1 Inner diameter
fW Wall friction force per unit volume
g Gravity constant
h Specific enthalpy
l Length or height
m Mass flow
p Pressure
P Pressure drop P Perimeter
Q Heat flux wall to fluid
Qest Heat flux outside to absorber
s Slip
S Energy sources
Sheat Specific heat generation rate
SM Momentum sources
τ Time
Δt Time step size
T Temperature
w Inner energy
v Volume
w Velocity
wli Relative velocity liquid and steam
wr Velocity of interphase mass transfer rate
x Coordinate along absorber
xext Flow quality
Δx Spatial resolution
α Steam void fraction
oh HTC Heat transfer coefficient
λ Thermal conductivity
λD Darcy-Weissbach friction factor
ρ Density
τi Interfacial shear per unit volume
ψ Interphase mass exchange per unit volume

Subscripts

F Fluid
i Interphase
l Liquid
m Mixture
v Steam
W Wall
ψ Interphase mass exchange
Acronyms

ATHLET  System code
DISE  Direct Solar Steam
Diss Dyn  Modelica library within Dymola
DSG  Direct Steam Generation
Dymola  Dynamic Modeling Laboratory
FEBE  Equation Solver (Forward-Euler, Backward-Euler)
GCSM  General Control Simulation Module

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Nuclear technologies such as fission and fusion reactors, including associated waste storage and disposal, rely on the availability not only of nuclear fuels but also of advanced structural materials. Various techniques have been developed to measure material properties at the microscopic and macroscopic level. Neutron scattering has played an important role in studying the structure and dynamics of condensed matter. The special nature of neutron interaction with matter provides important data which is complementary and supplementary to data gathered through other techniques.

The substantial penetration depth and selective absorption of neutrons make them a powerful tool in the non-destructive testing of materials with large and bulky samples. Residual stress formed in a material during manufacturing, welding, utilization or repairs can be investigated by means of neutron diffraction. In fact neutron diffraction is the only non-destructive testing method which can facilitate three-dimensional mapping of residual stress in a bulk component. Such studies are important in order to improve the quality of engineering components in production and to optimize design criteria in applications. The technique has applications in nuclear technology such as testing pipes and tubes, weld joints or structures under various conditions representative of those which might be experienced in service.

The IAEA conducted a Coordinated Research Project (CRP) on the Development and Application of the Techniques of Residual Stress Measurements in Materials (2006–2009). This project relied on the participation of practitioners from highly specialized user facilities from various Member States. The CRP objectives, among others, were:

- To optimize neutron beams for residual stress measurement using modern simulation techniques;
- To enhance beam intensity using modern neutron optics;
- To develop and test standardized procedures for the comparison of data from various instruments.

This publication is the main output of the project, and its purpose is to relate guidance on the basic principles, requirements, preparation, design, execution and standardization of residual stress measurements using neutron beams in a single publication. The publication will promote the use of neutron beams in residual stress measurements both at the microscopic and the macroscopic scale; facilitate preparation, design and standardization processes at less well equipped smaller research centres around the world; and offer guidance for young researchers and graduate students new to the field.

This report consists of nine sections including references. Section 2 defines the terms and techniques discussed in the report. Section 3 includes details of experimental techniques, while Section 4 describes associated equipment and instrumentation and their commissioning, calibration and control as well as data acquisition. Section 5 is dedicated to data analysis and interpretation. Section 6 of the report provides a number of selected examples for applications of residual stress measurements and Section 7 discusses future trends for development and use of this powerful technique. In addition, Annex I contains complete information on a number of round robin tests with standard samples and some results reported by the IAEA project participants. Finally, information on a dozen residual stress instruments worldwide and their characteristics is provided in Annex II.