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Low-order aquifer thermal energy storage model for geothermal system simulation

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Abstract

This paper presents a low-order aquifer thermal energy storage (ATES) model for simulation of combined sub-surface and above-surface energy systems. The model is included in the Modelica IBPSA Library, which is a free open-source library with basic models for building and district energy and control systems. The model uses a lumped-component method, in which the transient conductive-convective heat and mass transfer equation is radially discretized. To verify the accuracy of the model, we present an inter-model comparison from a simulation test suite. Results show that the Modelica ATES model is in good agreement, with a normalized mean bias error for yearly variation of aquifer temperatures of 1.6×10^{-2} and 9×10^{-5} at 1 m and 10 m distance from the well.

Keywords: Aquifer thermal energy storage, Thermodynamics, IBPSA library

1 Introduction

Buildings account for approximately 30% of global energy consumption and are responsible for a significant portion of greenhouse gas emissions (IEA 2022). As populations and urbanization continue to grow, the energy demands of buildings are also increasing. Hence, to limit climate change, it is important to move away from using fossil fuels for heating and cooling of buildings.

Thermal energy storage is a key technology to increase renewable energy utilization. Thermal storage refers to the temporary storage of thermal energy, which can be used later to meet heating and cooling demands. By integrating thermal storage into building energy systems, it is possible to shift the energy demand daily from peak hours to off-peak hours, when energy is cheaper and often more sustainable, or seasonally to shift heat availability from summer to winter. This leads to significant reductions in carbon emissions, as well as lower energy costs for building owners and occupants.

Aquifer Thermal Energy Storage (ATES) is a technology that improves sustainability of space heating and cooling for buildings through seasonal storage of heat in aquifers. An ATES system consists of at least two wells

which are coupled via a heat exchanger to exchange heat with the associated building. The basic operation of an ATES system is shown in Figure 1. In summer, cool groundwater is extracted from one well and circulated through the building system via heat exchangers or heat pumps. The water, which is heated during the process, is then injected into the other well (Dinçer et al. 2010). In winter the process is reversed. Since all the water from one well is re-injected into the other well, there is no net groundwater extraction.

ATES systems are a relatively modern technology. After engineering feasibility had been demonstrated in various projects, ATES technology was successfully established in Europe for both heating and cooling of buildings. Nowadays, more than 3000 ATES are implemented worldwide with 85% of the installations in the Netherlands and 10% in Sweden, Belgium and Denmark. Worldwide, ATES systems transfer a total amount of heat and cold that is estimated to exceed 2.5 TWh per year (Fleuchaus et al. 2018).

In early research studies on ATES, the focus revolved around solving technical, geochemical, and engineering obstacles. In subsequent years, the focus shifted towards improving system performances including the energy use of the above-surface plant facilities such as heat pumps, heat exchangers and cooling machines. Their performance is influenced by physical and chemical processes occurring underground. Predicting the behavior of these processes within a specific project often proves challenging with analytical calculations. Therefore, mathematical modeling took a pivotal role in the research and design of ATES systems.

Several ATES models and simulators have been presented in the literature. These are mostly developed using computational fluid dynamics software such as SHEMAT (Keller et al. 2020), FEFLOW (Trefry et al. 2007), MT3DMS (Bedekar et al. 2016), MODFLOW (Hughes et al. 2017). Such software enable an accurate prediction of underground conditions, but they have limited capabilities to integrate building simulation tools such as EnergyPlus, TRNSYS and Modelica, as only sophisticated co-simulations techniques can be used. Thus, a detailed

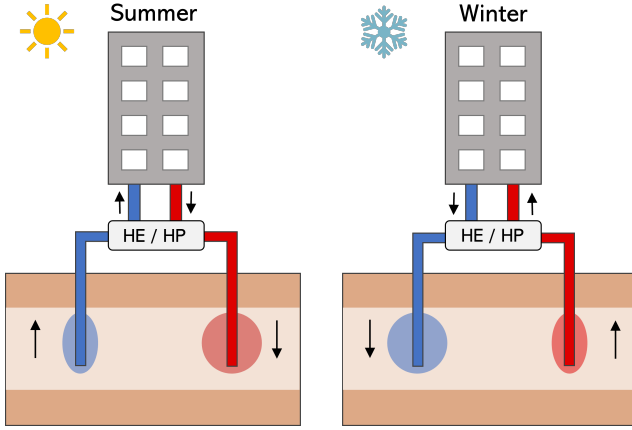


Figure 1. Basic working principle of an ATES system. The terms HE and HP stand respectively for heat exchanger and heat pump

performance analysis of an ATES connected to a building system typically requires knowledge in co-simulation, is computationally expensive, and is time consuming (Beernink et al. 2022; Bloemendal et al. 2018; Scalco et al. 2022).

Despite the fact that building systems (e.g. heat pumps, circulation pumps) dominate the primary energy use of ATES systems, only a few studies investigated the performance of ATES in conjunction with a detailed building system model. Bozkaya et al. (2018) developed a co-simulation method that combines COMSOL, MATLAB and TRNSYS. In this approach, COMSOL was used to model the ATES, TRNSYS to model the building and its heating, ventilation and air-conditioning (HVAC) system, and MATLAB acted as mediator to exchange information between the tools. Other studies (Kranz et al. 2013; Drenkelfort et al. 2015) used TRNAST, an ATES model developed for TRNSYS. The model is based on a finite-difference method and it relies on the assumptions that wells are thermally decoupled from each other. Tugores et al. (2015) describe a Modelica-based ATES model integrated into a district energy system model. The model was developed using a finite-volume approach and it was validated against a model simulated in COMSOL. However, this ATES model is not publicly available.

The literature review indicates that there is a lack of open-source, low-order ATES models that can enable fast and accurate geothermal system simulations integrating both above- and sub-surface system models.

This paper presents the development of an ATES model implemented in Modelica and to be included in the Modelica IBPSA Library (<https://github.com/ibpsa/modelica-ibpsa>). The Modelica IBPSA Library is a free open-source library with basic models that codify best practices for the implementation of models for building and district energy and control systems (Wetter, Treeck, et al. 2019). It is used as the basis of the four Modelica libraries AixLib (Müller et al. 2016), Buildings (Wet-

ter, Zuo, et al. 2014), BuildingSystems (Nytsch-Geusen et al. 2012) and IDEAS (Jorissen et al. 2018). Making available a free and open-source ATES model is expected to accelerate the uptake of ATES-based energy system solutions towards the decarbonization of the heating and cooling sector.

The paper is structured as follows: Section 2 presents the modeling approach, Section 3 presents an inter-model comparison for a test simulation case and the paper ends with concluding remarks.

2 Methodology

2.1 Modeling approach

To calculate aquifer temperature at different locations over time, the model solves simplified heat and mass transfer. The following assumptions were made to simplify the numerical modeling of ATES:

- The computational domain is homogeneous, i.e., material properties and physical parameters are constant across the entire domain.
- The aquifer is confined by two impermeable layers. Therefore, the vertical infiltration of water is neglected, i.e., the movement of water is only radial.
- All heat transfer is axial-symmetric, and there is no vertical heat transfer.
- Natural ground water flow is neglected. Movement of water is only driven by artificial pumping energy.

The model is based on the partial differential equation (PDE) for 1D conductive-convective transient radial heat transport in porous media

$$\rho c \frac{\partial T}{\partial t} = \lambda \frac{\partial^2 T}{\partial r^2} - u \rho_w c_w \frac{\partial T}{\partial r}, \quad (1)$$

where ρ is the density, c is the specific heat capacity, T is the temperature, r is the radius, λ is the thermal conductivity and u is the velocity. The subscript w indicates water. The first term on the right hand side of (1) describes the effect of conduction, while the second term describes convection.

The soil and its water content are assumed to be in thermal equilibrium, i.e. they can be described by the same temperature. With this assumption, the properties of the aquifer are calculated as a weighted average of the values for dry soil and water

$$\rho c = \phi \rho_w c_w + (1 - \phi) \rho_s c_s, \quad (2)$$

$$\lambda = \phi \lambda_w + (1 - \phi) \lambda_s, \quad (3)$$

where ϕ is the porosity [1] and subscript s denotes dry soil.

The geometric representation of the model is illustrated in Figure 2. The aquifer around the well is modeled as a radially symmetric disc.

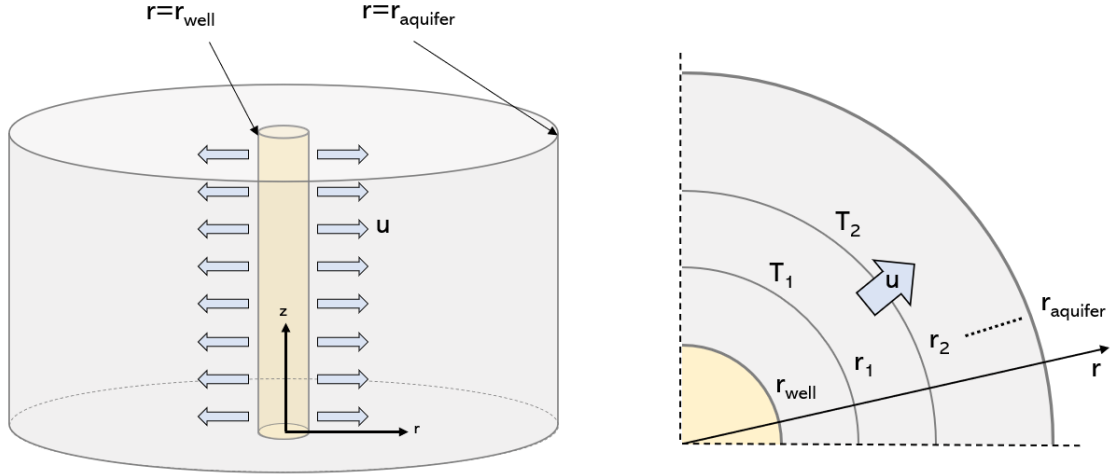


Figure 2. Geometric domain and discretization approach.

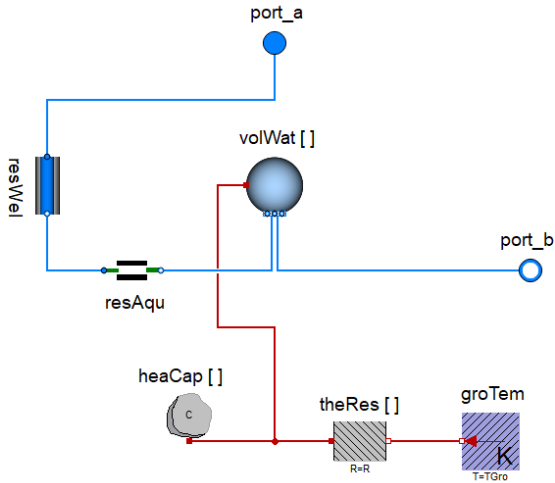


Figure 3. Modelica diagram of the ATEs model.

2.2 Modelica implementation

The model implementation in the Modelica language is based on a lumped-component approach as Modelica does not support describing PDEs (i.e., equations that involve the derivative of variables in spatial directions). Therefore, we spatially discretized the domain and implemented the heat transfer process in the aquifer using a series of thermal capacitances and resistances along the radial direction. The implementation uses an array of `HeatCapacitor` and `ThermalResistor` models, as shown in Figure 3. The fluid flow was modelled by adding a series of fluid volumes, which are connected to the thermal capacitances via heat ports. The fluid stream was developed using the model `IBPSA.Fluid.MixingVolumes.MixingVolume`. This model represents an instantaneously mixed volume, where potential and kinetic energy at the port are neglected.

The thermal capacitance of each cylindrical layer is

$$C_i = \rho c V_i, \quad (4)$$

where V_i is the volume of the i^{th} cylindrical layer. The thermal resistances are calculated as

$$R_i = \frac{\log\left(\frac{r_{c,i}}{r_{c,i-1}}\right)}{2\pi\lambda h}, \quad (5)$$

where $r_{c,i}$ is the radius to the center of the i^{th} cylindrical layer, $r_{c,i-1}$ is the radius to the center of the $(i-1)^{\text{th}}$ cylindrical layer, and h is the thickness of the aquifer.

Based on this lumped-component approach, the heat balance for the i^{th} cylindrical layer is

$$C_i \frac{dT_i}{dt} = \frac{T_{i+1} - T_i}{R_{i+1}} + \frac{T_{i-1} - T_i}{R_i} + \dot{m}_w c_w \begin{cases} (T_{i-1} - T_i), & \text{if } \dot{m}_w \geq 0, \\ (T_i - T_{i+1}), & \text{otherwise,} \end{cases} \quad (6)$$

where \dot{m}_w is the water mass flow rate. The first and second term on the right hand side of (6) represent the heat conduction to neighboring layers, while the third term represents the heat convection caused by the movement of water.

Each cylindrical layer is spaced according to an expansion coefficient. This number is used to increase the size of the cylindrical layers from the well to the outer boundary of the aquifer.

The friction losses are computed using a power law model expressed by

$$\dot{m}_w = k \Delta p^m, \quad (7)$$

where k is a flow coefficient, Δp is the pressure difference, and m is the flow exponent. The flow coefficient is based on one data point of mass flow rate and pressure difference, and a given flow exponent.

3 Numerical experiments

3.1 Simulation setup

Ideally, the validation of a mathematical model would include comparison against measurements. However, mea-

asuring an ATEs system, retrieving data, and analyzing them is a complex and costly task, and we had no such data available. Therefore, we conducted an inter-model comparison, using a simulation test suite developed by Mindel et al. (2021). This test suite comprises a set of cases to assess the thermo-hydraulic modelling capabilities of various geothermal simulators.

The comparison was carried out with respect to the test case called "TC2 - well-test comparison". The main goal of TC2 is to compare aquifer temperatures under a typical operation of an ATEs system consisting of injection, falloff, drawdown, and build-up. Such a sequence represents an idealized operation of a seasonal storage system.

The injection phase represents the charging period, while the drawdown phase represents the discharge period. Intermediate phases of falloff and build-up represent periods of storage or inactivity. The overall operational period is one year, and the sequence of the different phases is the following:

1. **Injection:** Water is pumped at $\dot{m}_w = 1 \text{ kg s}^{-1}$ and $T_{inj} = 120^\circ\text{C}$ for 120 days.
2. **Falloff:** Well is shut-in, $\dot{m}_w = 0 \text{ kg s}^{-1}$, for 60 days.
3. **Drawdown:** Water is pumped at $\dot{m}_w = -1 \text{ kg s}^{-1}$ for 120 days.
4. **Build-up phase:** Well is shut-in, $\dot{m}_w = 0 \text{ kg s}^{-1}$, for 65.25 days.

A list of relevant input parameters used for the simulations are shown in Table 1.

Table 1. Simulation input specification summary.

Parameter	Value	Unit
Porosity	0.2	[1]
Soil density	2680	kg m^{-3}
Soil thermal conductivity	2.8	$\text{W m}^{-1} \text{K}^{-1}$
Soil specific heat capacity	833	$\text{J kg}^{-1} \text{K}^{-1}$
Wellbore radius	0.1	m
Domain radius	2400	m
Domain height	200	m
Initial temperature	34	$^\circ\text{C}$
Injection temperature	120	$^\circ\text{C}$

For comparative purposes, temperature values were recorded via virtual probes located at $r = \{1, 10\} [m]$ for $t = \{0, 50, 100, 150, 200, 250, 310, 365.25\} [days]$.

3.2 Result comparison

Figure 4a shows the temperature vs. time comparison for the first probe, located at $r = 1 \text{ m}$. Overall, the simulation results of the Modelica model (named *IBPSA_Mod* in the graph) are in good agreement with the other simulators. As stated in Mindel et al. (2021), the discrepancy between

the initial value of temperature for *Tough3*, *MOOSE* and the other simulators is due to the different injection conditions. These simulators do not use an enthalpy source-type or a Neuman boundary condition but they use a Dirichlet boundary condition. It can also be observed that the tool *CODE_BRIGHT* presents a time delay.

Figure 4b shows the temperature vs. time comparison for the second probe, located at $r = 10 \text{ m}$. Also in this case, the Modelica model provides simulation results that are in good agreement with the other simulators. Data from *Tough3* have been omitted from Figure 4b as they largely differ from the other tools.

Note that the test suite includes temperature comparisons also for probes located further away from the well ($r > 10 \text{ m}$). However, at such locations, only a small numerical fluctuation can be observed, which is about $\pm 0.01^\circ\text{C}$ around the initial temperature of 34°C . Therefore, these test cases have not been included in this work.

To quantitatively compare the simulation results, we normalize the temperatures by their driving potential, and use the Mean Bias Error (MBE), applied to the point-to-point difference between the model and a reference value. We normalized the temperatures using

$$\theta = \frac{T - T_{min}}{T_{max} - T_{min}}, \quad (8)$$

where T is the temperature of the simulation, T_{min} is equal to the initial conditions $T_{min} = 34^\circ\text{C}$, and $T_{max} = 120^\circ\text{C}$ is the temperature at which the water is injected.

The mean bias error is

$$MBE = \frac{\sum_{i=1}^n (\theta_{m,i} - \theta_{r,i})}{n}, \quad (9)$$

where the subscript m denotes the model value and r the reference value. For the reference values, we used the average of all other simulators, but removed the results from *Tough3*, *MOOSE* and *CODE_BRIGHT*, as they are seen as outliers due to different boundary conditions and time delay.

The results are shown in Table 2 and Table 3. For the probe located at $r = 1 \text{ m}$, the normalized MBE is 1.6×10^{-2} , while for the probe at $r = 10 \text{ m}$, it is 9×10^{-5} . Since both values are positive, it can be deduced that the Modelica model globally over-predict the results. The higher normalized MBE for the probe at $r = 1 \text{ m}$ is mostly due to the fact that the simulation results of the Modelica model lie on the high end of the temperature range across tools.

4 Conclusions

ATES is a technology that enables seasonal storage of thermal energy in the groundwater. Several ATEs models exist in literature, but these typically use computational fluid dynamics software, making it difficult to analyze the interactions between sub-surface and above-surface energy systems.

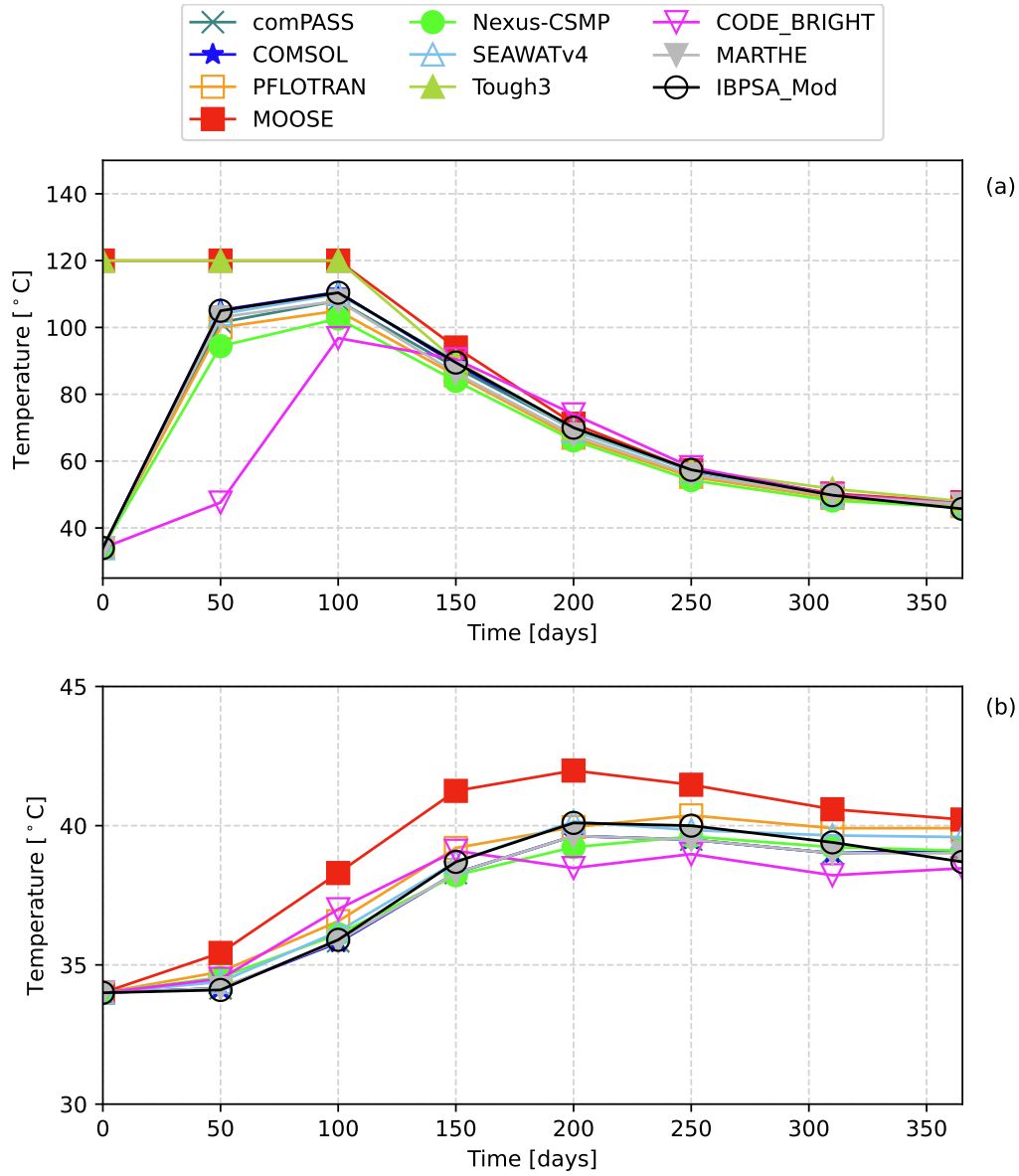


Figure 4. Temperature variation over time for the probes located at $r=1$ m (a) and $r=10$ m (b).

Table 2. Quantitative comparison for $r = 1$ m.

Time [d]	θ_m	θ_r	Error
0	0	0	0
50	8.3×10^{-1}	7.8×10^{-1}	4.2×10^{-2}
100	8.9×10^{-1}	8.5×10^{-1}	3.5×10^{-2}
150	6.5×10^{-1}	6.2×10^{-1}	2.7×10^{-2}
200	4.2×10^{-1}	4×10^{-1}	2×10^{-2}
250	2.7×10^{-1}	2.6×10^{-1}	1.5×10^{-2}
310	1.8×10^{-1}	1.8×10^{-1}	5.8×10^{-3}
365.25	1.4×10^{-1}	1.5×10^{-1}	-1.4×10^{-2}
			MBE= 1.6×10^{-2}

Table 3. Quantitative comparison for $r = 10$ m.

Time [d]	θ_m	θ_r	Error
0	0	0	0
50	1.2×10^{-3}	4×10^{-3}	2.8×10^{-3}
100	2.2×10^{-2}	2.4×10^{-2}	-1.9×10^{-3}
150	5.5×10^{-2}	5.2×10^{-2}	2.3×10^{-3}
200	7.1×10^{-2}	6.6×10^{-2}	4.9×10^{-3}
250	7×10^{-2}	6.6×10^{-2}	3.6×10^{-3}
310	6.3×10^{-2}	6.2×10^{-2}	6.4×10^{-3}
365.25	5.5×10^{-2}	6.1×10^{-2}	-6.4×10^{-3}
			MBE= 9×10^{-5}

We presented the development of a simplified ATES model to be included in the Modelica IBPSA Library. This is expected to facilitate the design, operation and control of ATES-based energy systems, as the ATES model can be directly connected to above-surface energy system models, typically by use of a heat exchanger or a heat pump.

The accuracy of the model was validated by performing an inter-model comparison using results from a simulation test suite. Results showed that the Modelica ATES model can predict aquifer temperatures with a good degree of accuracy. The normalized mean bias error at $r = 1\text{ m}$ and $r = 10\text{ m}$ distance from the well was 1.6×10^{-2} and 9×10^{-5} respectively.

Further work will focus on the validation of the model against measurements retrieved from a real-life ATES system. Moreover, a detailed application case study consisting of a full coupling between the ATES model and building energy system model will be developed and the model will be included in the Modelica IBPSA Library. In addition, a multi-well model will be developed to enable the connection of multiple wells within the same ATES system.

5 Data availability statement

The model is available from <https://github.com/ibpsa/modelica-ibpsa>, commit <https://github.com/ibpsa/modelica-ibpsa/commit/84f9135e737147fee779962a3b3f33ea40479657>. The validations were performed using commit <https://github.com/ibpsa/modelica-ibpsa/commit/b073350fe7952dc70ff3f60a014f4431ad3f5d43>.

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