Accelerating Numerical Analysis of Near-Critical CO_2 Flow Transients using a Pre-trained Property Network.

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1. Introduction

This study introduces and validates an enthalpy-based Implicit Continuous Eulerian (ICE) solver called "Near-Critical ICE Solver" (NICES) designed for the assessment of thermodynamic systems involving near-critical CO_2. Conventional methodologies, which rely on pressure and temperature as primary inputs, encounter challenges when dealing with CO_2 near its critical point due to its distinctive properties and frequent phase transitions. To address these challenges, this research advocates for the utilization of enthalpy as a more suitable mathematical foundation. The NICES approach leverages the homogeneous equilibrium model alongside the Span and Wagner equations [1] of property model for CO_2. Through its application, this solver showcases enhanced numerical robustness and computational efficiency when compared to semi-implicit calculation techniques. In this approach, most serious bottle neck is revealed that computational time to calling property packages. To overcome this bottle-neck, pre-trained network-based property model is proposed for accelerating the numerical simulation. This assertion is substantiated through analyses of frictionless heated pipe scenarios involving phase shifts in proximity to the critical point. Notably, the enthalpy-centered NICES platform adeptly predicts thermohydraulic behaviors, including scenarios with multiphase flows, obviating the necessity for additional specialized two-phase flow models. The deployment of NICES is poised to be instrumental in the investigation of mechanical energy storage systems, transcritical CO_2 cycles and supercritical steam systems.

2. Methodology

2.1 Governing Equations

It is crucial to consider equations with compressible fluids to analyze thermodynamic systems on the development platform. Therefore, the primary governing equation used in this study is adopted from previous research conducted by Plant Dynamics Code (PDC) [2]. The dynamic behavior of the flow in the pipe can be described by three conservative equations: continuity, momentum, and energy. Furthermore, according to the previous research by Hewitt et al. [3] and Yan et al. [4], conservation equations can be written in simplified partial differential equation form as shown in Equations (1)–(3).

Continuity, Equation (1)

$$\frac{\partial \bar{\rho}}{\partial t} = \frac{\dot{m}_{in} - \dot{m}_{out}}{A \Lambda x}$$

Momentum, Equation (2)

$$\frac{\partial \bar{m}}{\partial t} = (P_{in} - P_{out}) \frac{A}{\Delta x} - 2f \frac{\bar{m}^2}{A \bar{\rho} D_h}$$

Energy, Equation (3)

$$\frac{\partial \bar{h}}{\partial t} = \frac{1}{\bar{\rho} A \Delta x} \left[\dot{m}_{in} \left(h_{in} - \bar{h} \right) - \dot{m}_{out} \left(h_{out} - \bar{h} \right) + q' \Delta x \right]$$

2.2 Implicit Continuous Eulerian method

The ICE technique presents a computational methodology employed for the evaluation of transient thermohydraulic systems. Distinguished as a semi-implicit approach, this method amalgamates the merits inherent to both implicit and explicit methodologies.

Typically, the calculation procedure for ICE methods unfolds through the subsequent steps:

1. Express the momentum equation by utilizing pressure differentials.
2. Formulate the energy equation incorporating momentum data from the upcoming time step and the prevailing energy data. During this phase, explicit components are incorporated. In instances where numerical instability emerges, an alternative approach involves representing the energy equation with the pressure from the following time step.
3. Resolve the pressure matrix and iteratively compute its values until convergence is achieved.

In this research, Enthalpy and Pressure are selected as basis for these numerical simulations.

2.3 Deep Neural Network based property model

One of the most significant challenges in simulating near-critical fluid transients revolves around computation time. The profiling outcomes are presented in Table 1, outlining the performance breakdown of the developed simulator during a 1000-second-long transient simulation, utilizing the scenario elucidated in Chapter 3 as an example. The profiling analysis is carried out employing the cProfile package.

As articulated in the introductory section, the findings in Table 1 reveal that the primary bottleneck in the computation of trans/supercritical CO_2 transient analyses lies in the time spent on calling properties from the equation of states (EOS). Notably, over 97% of the computation time is devoted to invoking EOS modules. This pronounced allocation of time is attributed to the intricate nature of the Span-Wagner EOS [1], which necessitates iterative solutions, particularly in calculations near the critical point.

Table 1. Profiling result of the developed enthalpy-based ICE simulator for 1000sec-long transient simulation.

Number of call module	Time consumption (sec)	Time consumption / Total time (%)	Module name
1	**1040.897**	**97.00485352**	CoolProp.pyx:377(PropsSI) - **EOS Module**
1	12.832	1.195859226	Profiling_Fluid_block.py:16(test)
1331748	5.061	0.471652396	linalg.py:476(inv)
1331748	1.902	0.177254072	{method 'dot' of 'numpy.ndarray' objects}
1331748	1.182	0.110154739	linalg.py:135(_commonType)
2257203	1.145	0.106706578	{built-in method CoolProp.CoolProp.PropsSI} - **EOS Module**
6771609	0.962	0.089652165	CoolProp.pyx:109(iterable) - **EOS Module**
2257203	0.798	0.074368428	CoolProp.pyx:377(PropsSI (wrapper)) - **EOS Module**
361152	0.597	0.05563653	iostream.py:518(write)
1331748	0.583	0.054331821	<__array_function__ internals>:2(inv)
9028812	0.579	0.053959047	stringsource:13(__pyx_convert_string_from_py_std__in_string)
(Omitted below)			

To overcome this bottle-neck, this research proposes the way to implement pre-trained property network to avoid direct property calculation. In the Implicit Continuous Eulerian methodology, there are three parts that require property calls: $\rho(H,P)$, $\frac{\partial \rho}{\partial P}|_H\,(H,P)$, and $\frac{\partial \rho}{\partial H}|_P\,(H,P)$. Since $\frac{\partial \rho}{\partial P}|_H$ and $\frac{\partial \rho}{\partial H}|_P$ are derivable functions from ρ, we utilized the approach of training ρ on H and P, and deriving $\frac{\partial \rho}{\partial P}|_H$ and $\frac{\partial \rho}{\partial H}|_P$ via numerical differentiation. So, for this example, it is trained that a database of densities based on pressure and enthalpy.

3. Experiment

To assess the effectiveness of the proposed methodology, two illustrative scenarios involving heated pipe flows with phase transitions near critical points are employed. The first scenario, denoted as Case 1, serves as an instance of a phase transition from a liquid to a supercritical state. Meanwhile, Case 2 presents an example of a phase transition from liquid to gas. These scenarios are visually depicted in Figure 1.

The problem revolves around the flow within a frictionless, heated pipe. The initial premise assumes a steady state up until t = 0, where the system experiences no heating and operates with an inlet flow rate of 1 kg/s. At this pivotal moment, there is a sudden surge in the inlet flow rate to 1.1 kg/s, coinciding with the initiation of wall heating at a rate of 165 kW/m. Under the provided conditions, the fluid states are proximate to the critical point. During the transient phase, a remarkable phenomenon takes place within the heated pipe, leading to either a supercritical state (Case 1) or a gaseous state (Case 2). The trajectories of these processes in the T-S diagram during the steady state are showcased in Figure 2. Additionally, the diagram visually highlights that in Case 2, the transition from liquid to gas transpires through the boiling point.

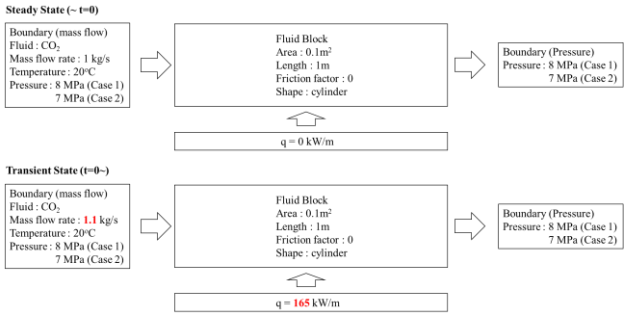

Figure 1. Simple modulization of example problem Case 1 and 2

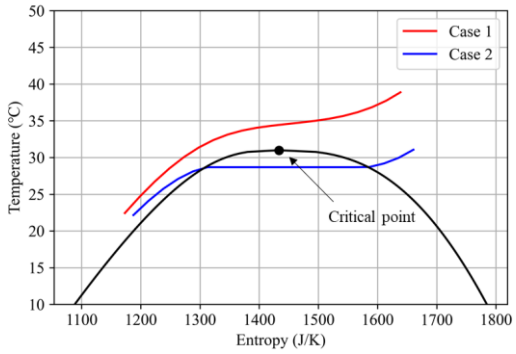

Figure 2. Pathway of processes Cases 1 and 2 at steady state in T–S diagram.

Figure 3 shows the result in Case 1 and Figure 4 shows Case 2's. Result shows the developed simulator

progress near-critical phase-changing simulation robustly.

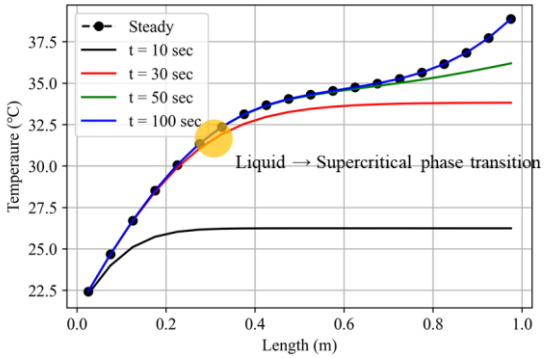

Figure 3. Temperature and mass flow rate development through the time of Case 1.

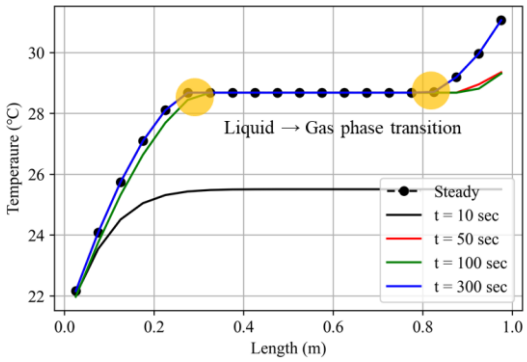

Figure 4. Temperature and mass flow rate development through the time in Case 2.

4. Conclusion and Further works

In this extended abstract, we show that the bottle-neck for transient simulation of near-critical fluids is the time it takes to call the property module, and we propose the idea of using a pre-trained property network as a way to solve this problem. It is also developed an enthalpy-based ICE simulator to increase the numerical stability of the simulation and verify the idea with the simulator until transaction meeting.

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